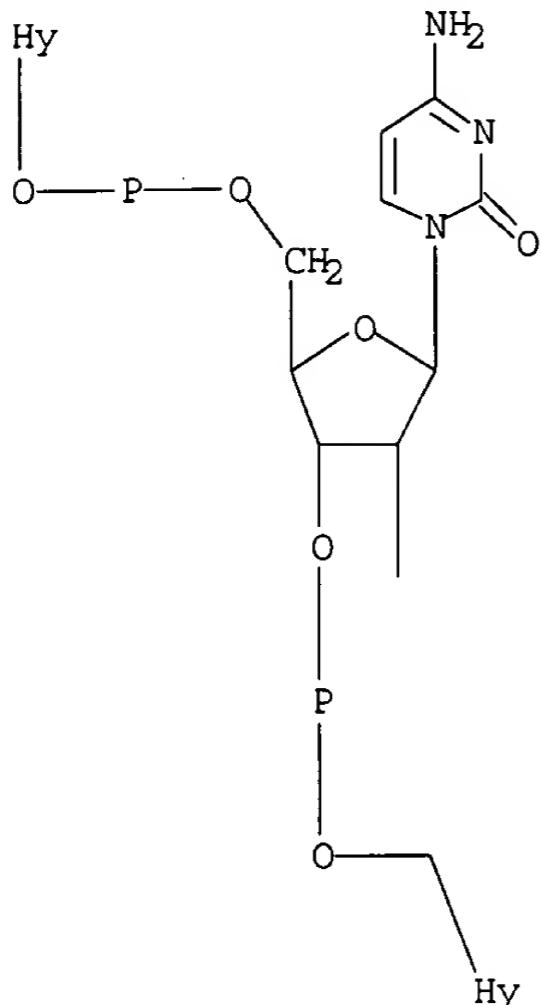


Page 1

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L1 STR



Structure attributes must be viewed using STN Express query preparation.

L2 14 SEA FILE=REGISTRY SSS FUL L1

L3 4 SEA FILE=CAPLUS ABB=ON PLU=ON L2

=> d his

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L1 STRUCTURE uploaded

L2 14 L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 18:06:27 ON 12 JUN 2003

L3 4 L2

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L3 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:127033 CAPLUS

DOCUMENT NUMBER: 136:386341

TITLE: 2'-Ethynyl-DNA: synthesis and pairing properties

AUTHOR(S): Buff, Rolf; Hunziker, Jurg

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Bern, Bern, CH-3012, Switz.

SOURCE: Helvetica Chimica Acta (2002), 85(1), 224-254

CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 2-Ethynyl-DNA was developed as a potential DNA-selective oligonucleotide analog. The synthesis of 2'-arabino-ethynyl-modified nucleosides was achieved starting from properly protected 2'-ketonucleosides by addition of lithium (trimethylsilyl)acetylide followed by reduction of the tertiary alc. After a series of protecting-group manipulations, phosphoramidite building blocks suitable for solid-phase synthesis were obtained. The synthesis of oligonucleotides from these building blocks was successful when a fast deprotection scheme was used. The pairing properties of 2'-arabino-ethynyl-modified oligonucleotides can be summarized as follows: The 2'-arabino-ethynyl modification of pyrimidine nucleosides leads to a strong destabilization in duplexes with DNA as well as with RNA. The likely reason is that the ethynyl group sterically influences the torsional preferences around the glycosidic bond leading to a conformation not suitable for duplex formation. If the modification is introduced in purine nucleosides, no such influence is observed. The pairing properties are not or only slightly changed, and, in some cases (deoxyadenosine homo-polymers), the desired stabilization of the pairing with a DNA complementary strand and destabilization with an RNA complement is observed. In oligonucleotides of alternating deoxycytidine-deoxyguanosine sequence, the incorporation of 2'-arabinoethynyl deoxyguanosine surprisingly leads to the formation of a left-handed double helix, irresp. of salt concentration. The rationalization for this behavior is that the ethynyl group locks such duplexes in a left-handed conformation through steric blockade.

IT 231623-33-9P 424822-71-9P 424822-72-0P  
424822-78-6P 424822-79-7P

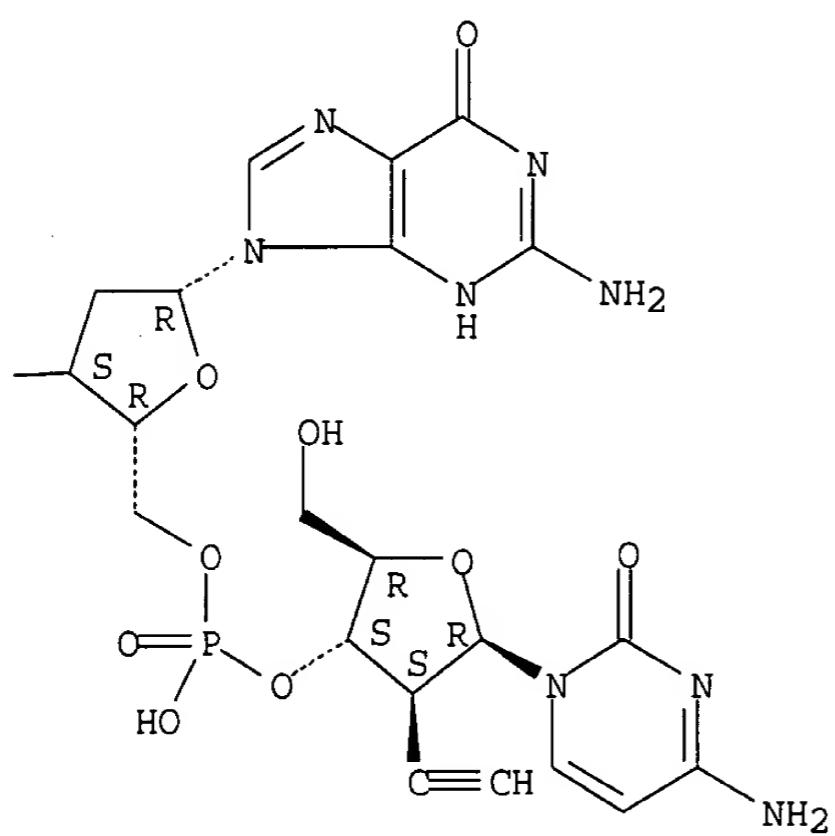
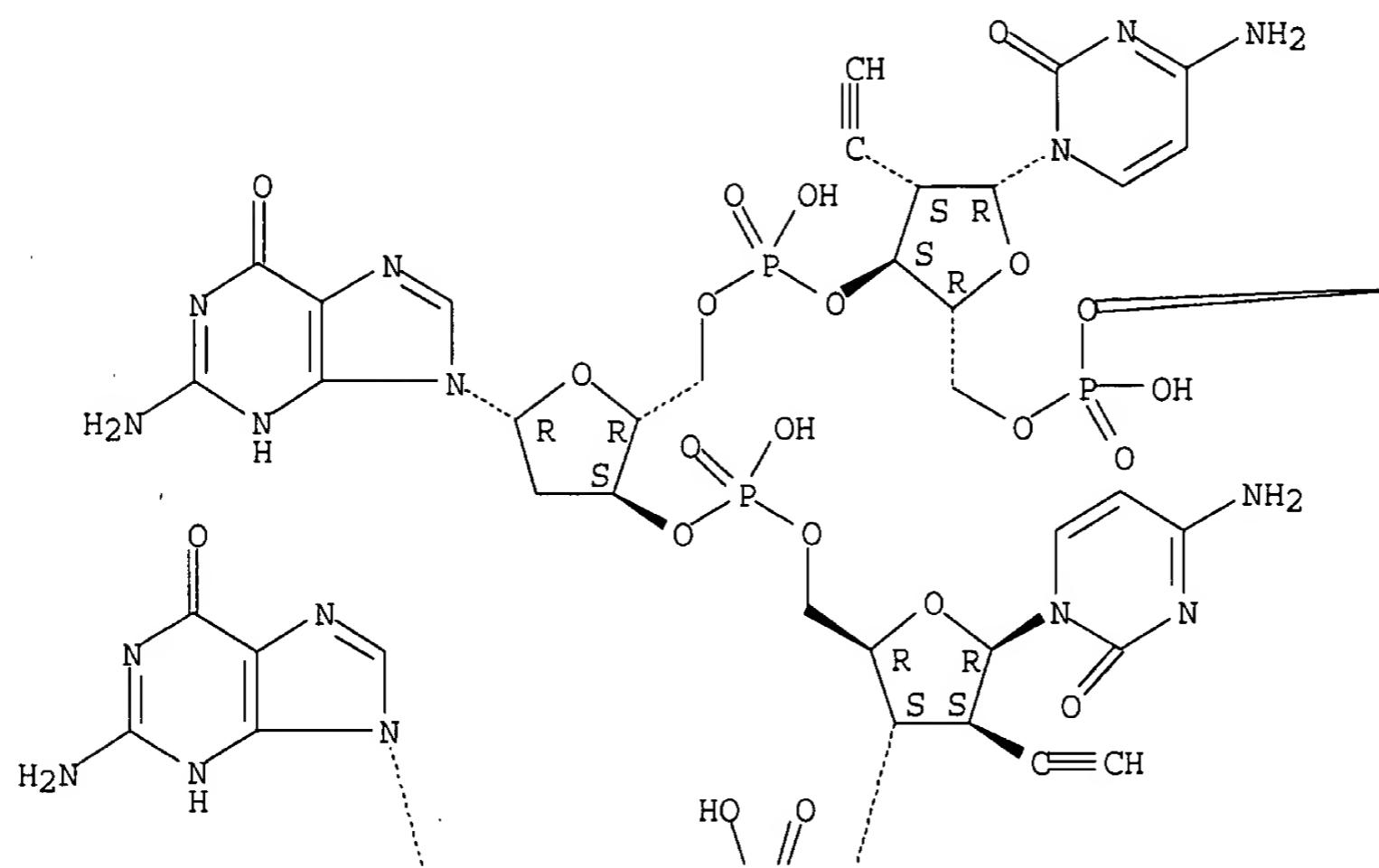
RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation);  
RACT (Reactant or reagent)

(preparation of 2'-Ethynyl-DNA to be used in the synthesis and pairing properties of DNA and RNA duplexes)

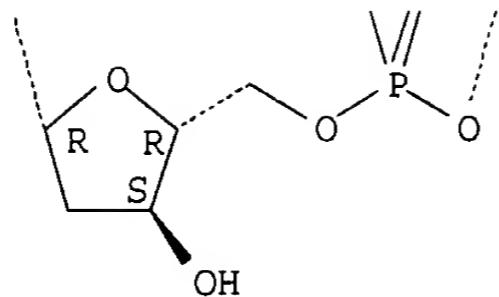
RN 231623-33-9 CAPLUS

CN Guanosine, 2'-deoxy-2'-ethynyl- $\beta$ -D-arabino-cytidylyl-(3'→5')-  
2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl- $\beta$ -D-arabino-  
cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-  
ethynyl- $\beta$ -D-arabino-cytidylyl-(3'→5')-2'-deoxy- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.



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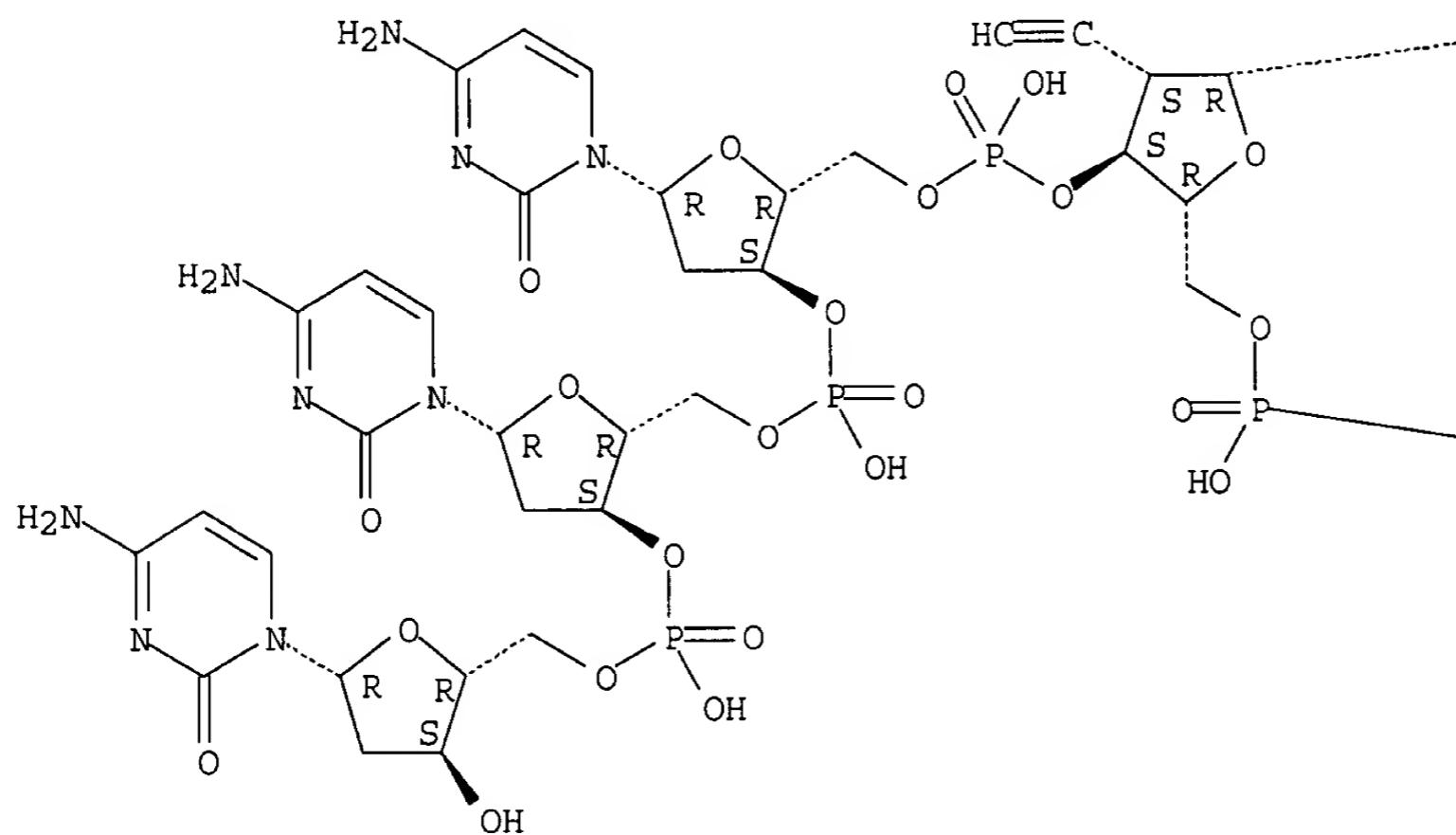


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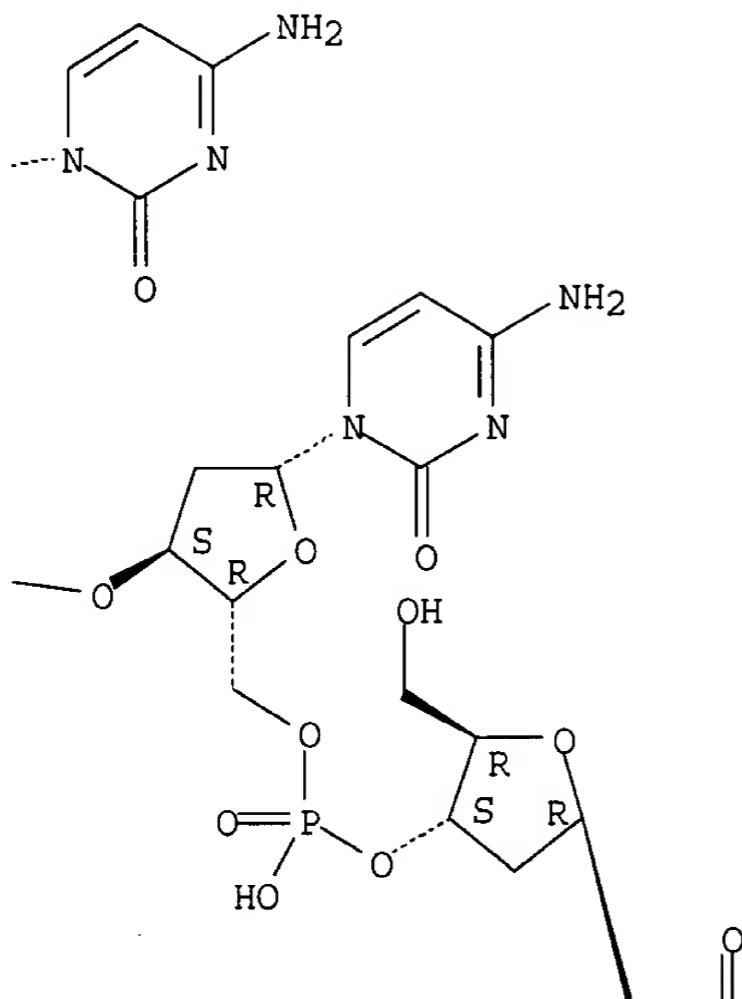
CN Cytidine, 2'-deoxycytidyl-(3'→5')-2'-deoxycytidyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidyl-(3'→5')-2'-deoxycytidyl-(3'→5')-2'-deoxycytidyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

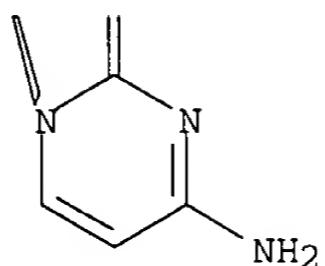
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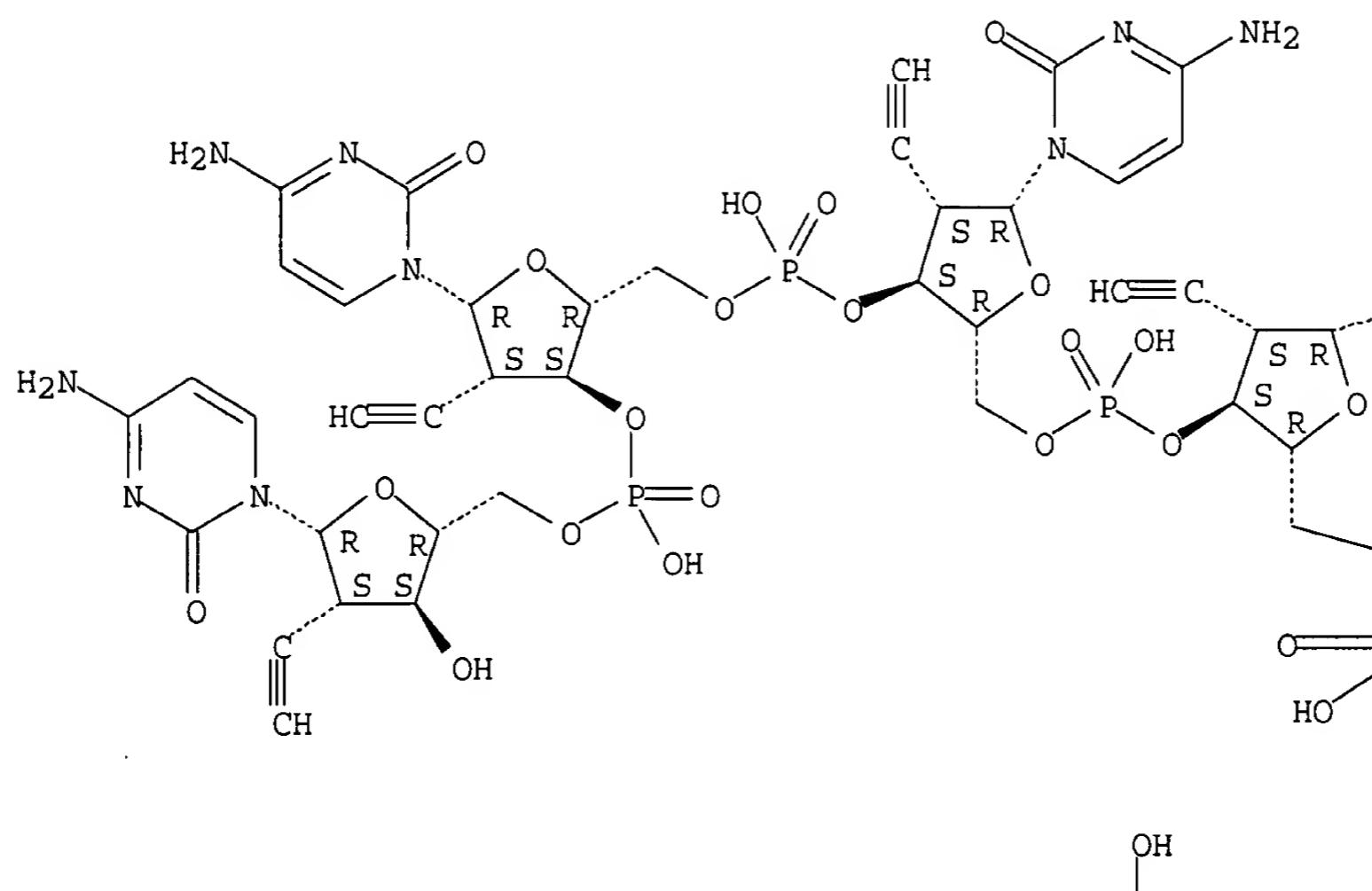


RN 424822-72-0 CAPLUS

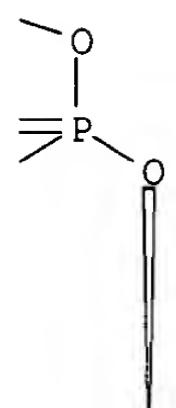
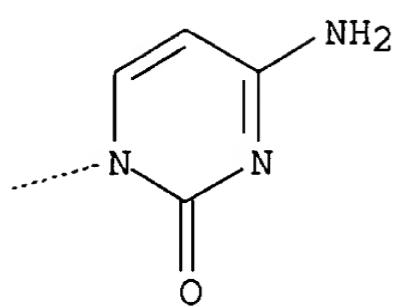
CN  $\beta$ -D-arabino-Cytidine, 2'-deoxy-2'-ethynyl- $\beta$ -D-arabino-cytidyl-(3'  $\rightarrow$  5')-2'-deoxy-2'-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

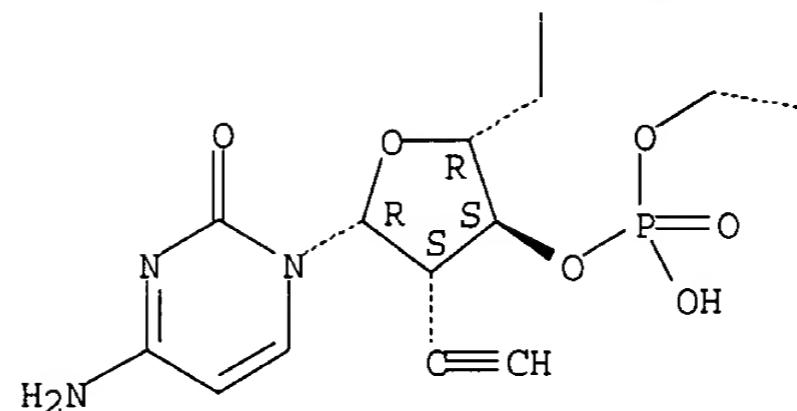
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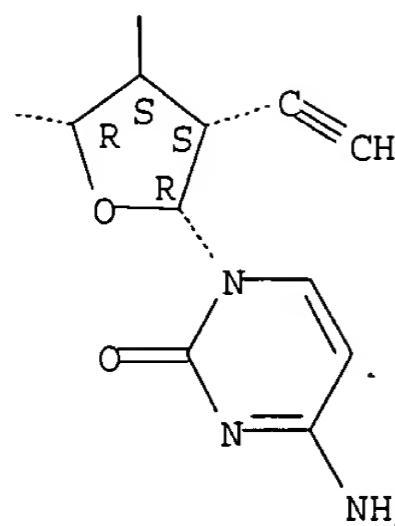
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PAGE 2-A



PAGE 2-B

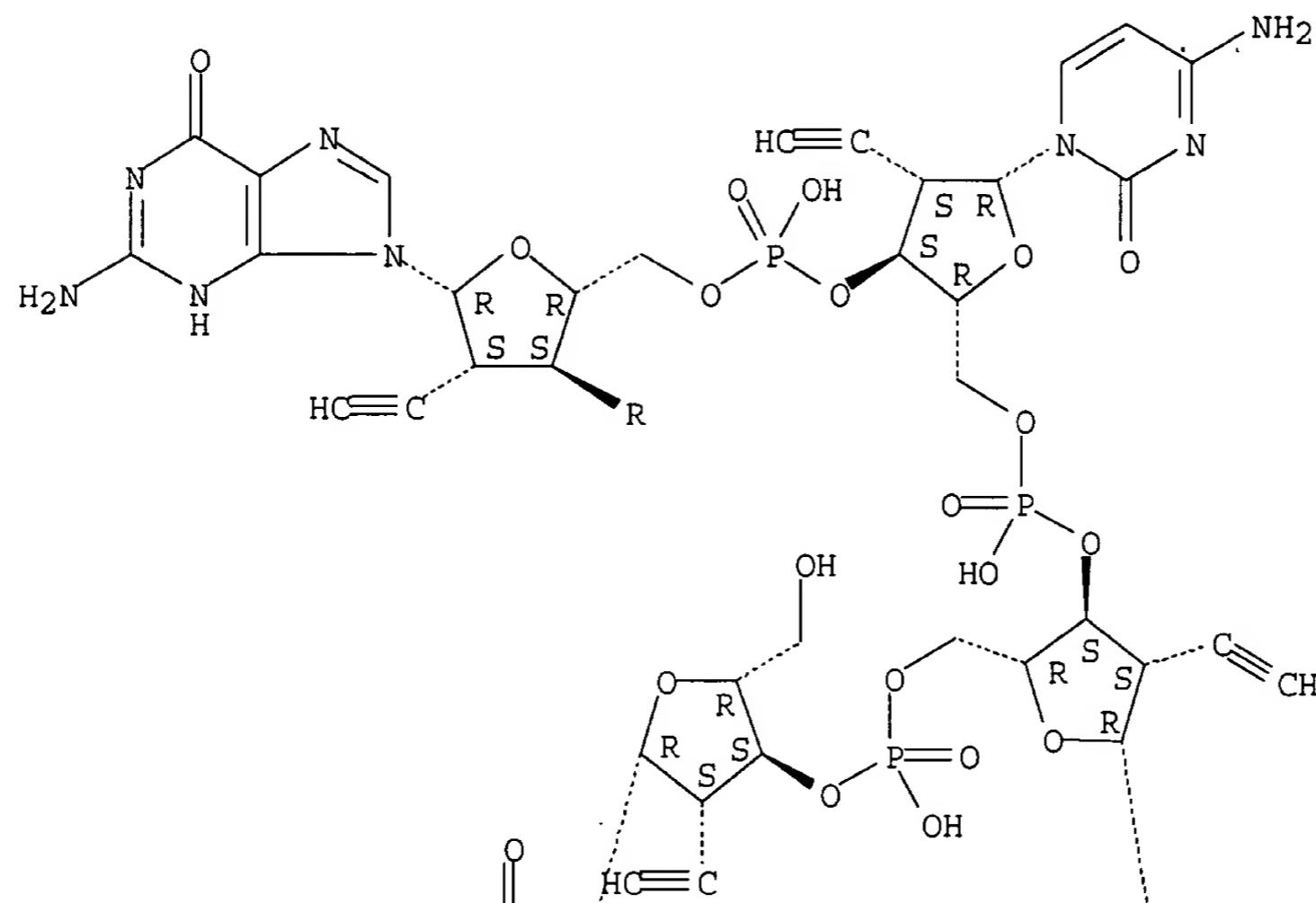


RN 424822-78-6 CAPLUS

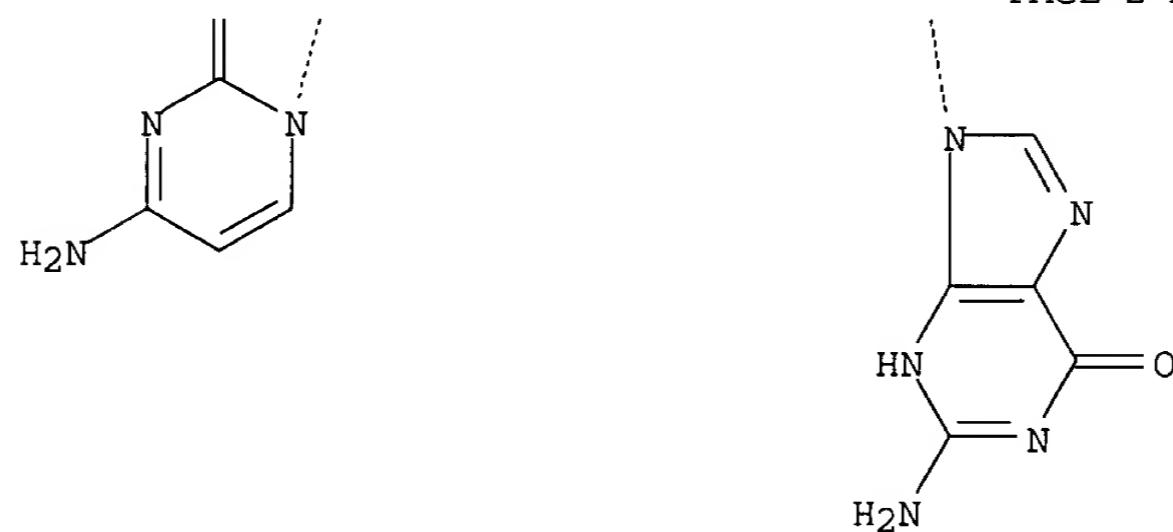
CN  $\beta$ -D-arabino-Guanosine, 2'-deoxy-2'-ethynyl- $\beta$ -D-arabino-cytidylyl-  
(3'  $\rightarrow$  5')-2'-deoxy-2'-ethynyl- $\beta$ -D-arabino-guanylyl-  
(3'  $\rightarrow$  5')-2'-deoxy-2'-ethynyl- $\beta$ -D-arabino-cytidylyl-  
(3'  $\rightarrow$  5')-2'-deoxy-2'-ethynyl- $\beta$ -D-arabino-guanylyl-  
(3'  $\rightarrow$  5')-2'-deoxy-2'-ethynyl- $\beta$ -D-arabino-cytidylyl-  
(3'  $\rightarrow$  5')-2'-deoxy-2'-ethynyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

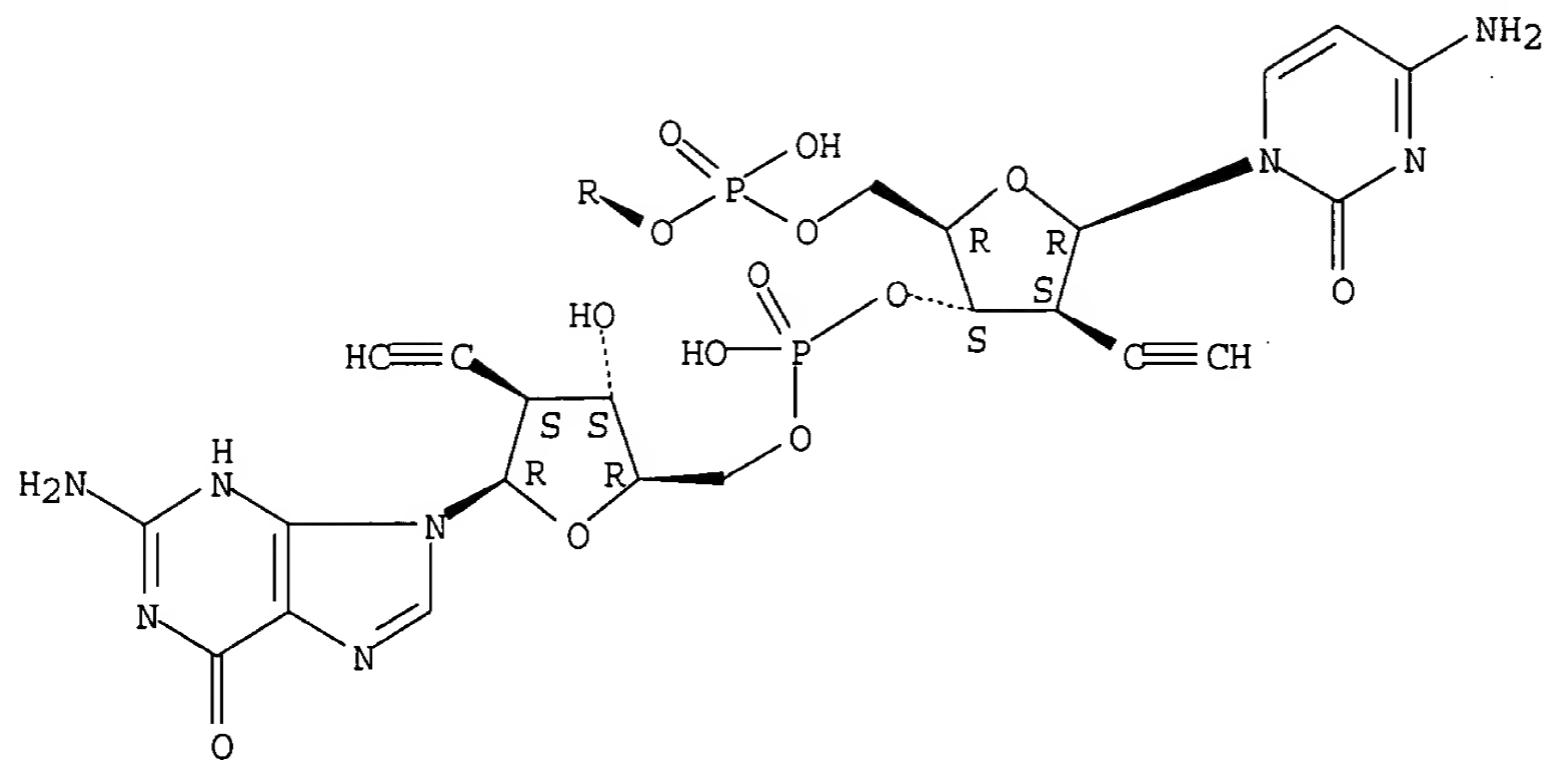
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PAGE 2-A



PAGE 3-A

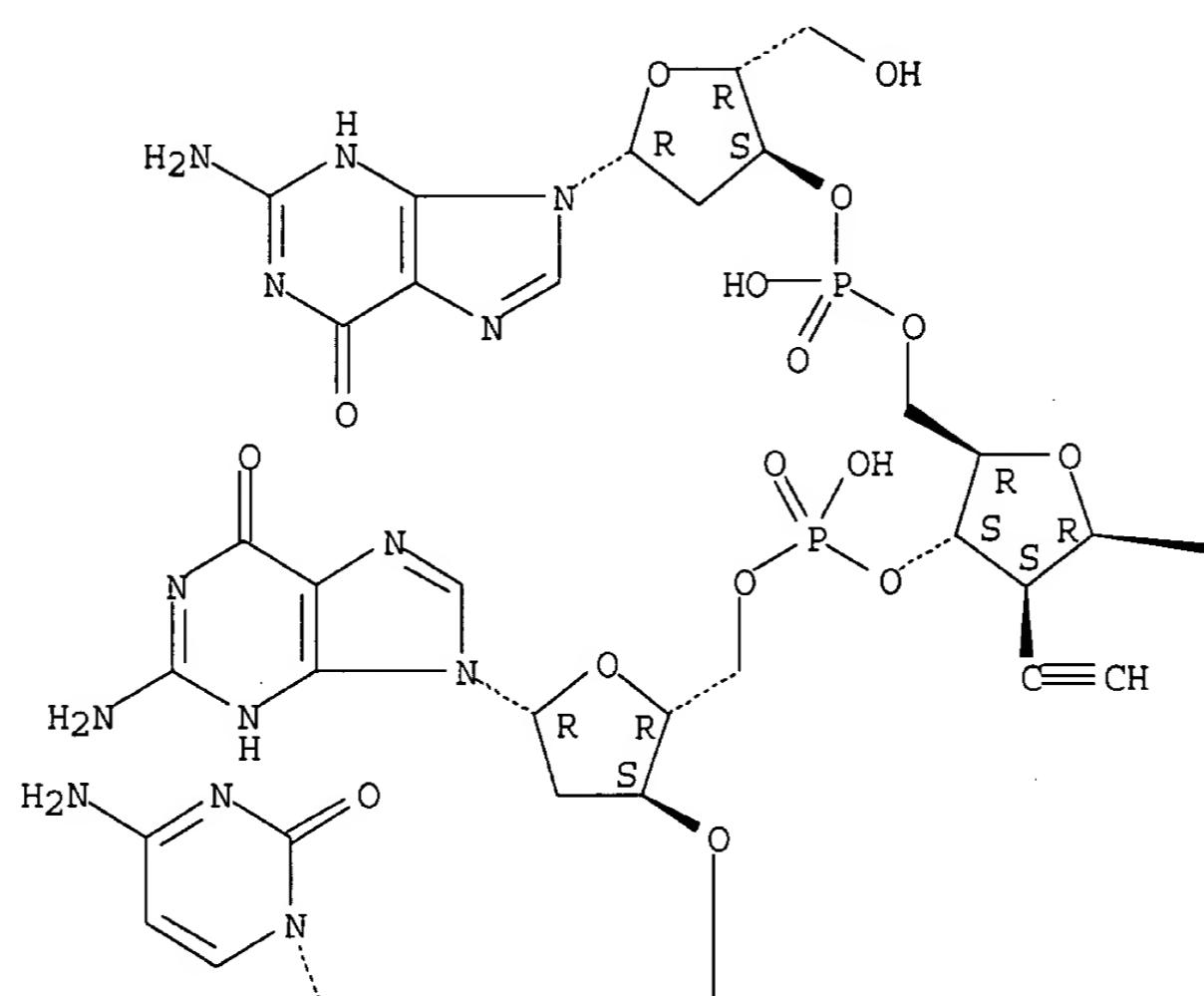


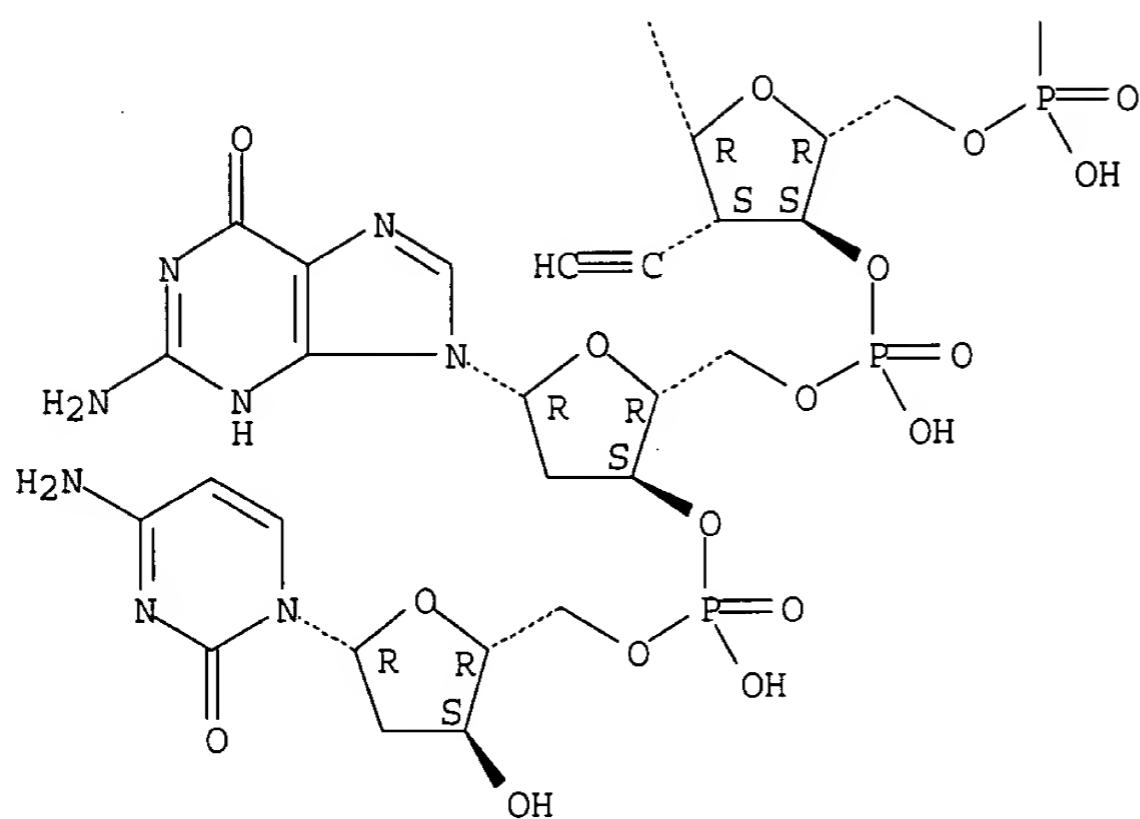
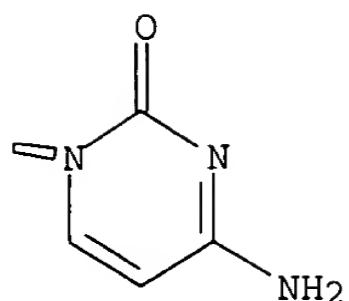
RN 424822-79-7 CAPLUS

CN Cytidine, 2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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IT 231623-33-9DP, self-complementary 424822-80-0P

424822-82-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

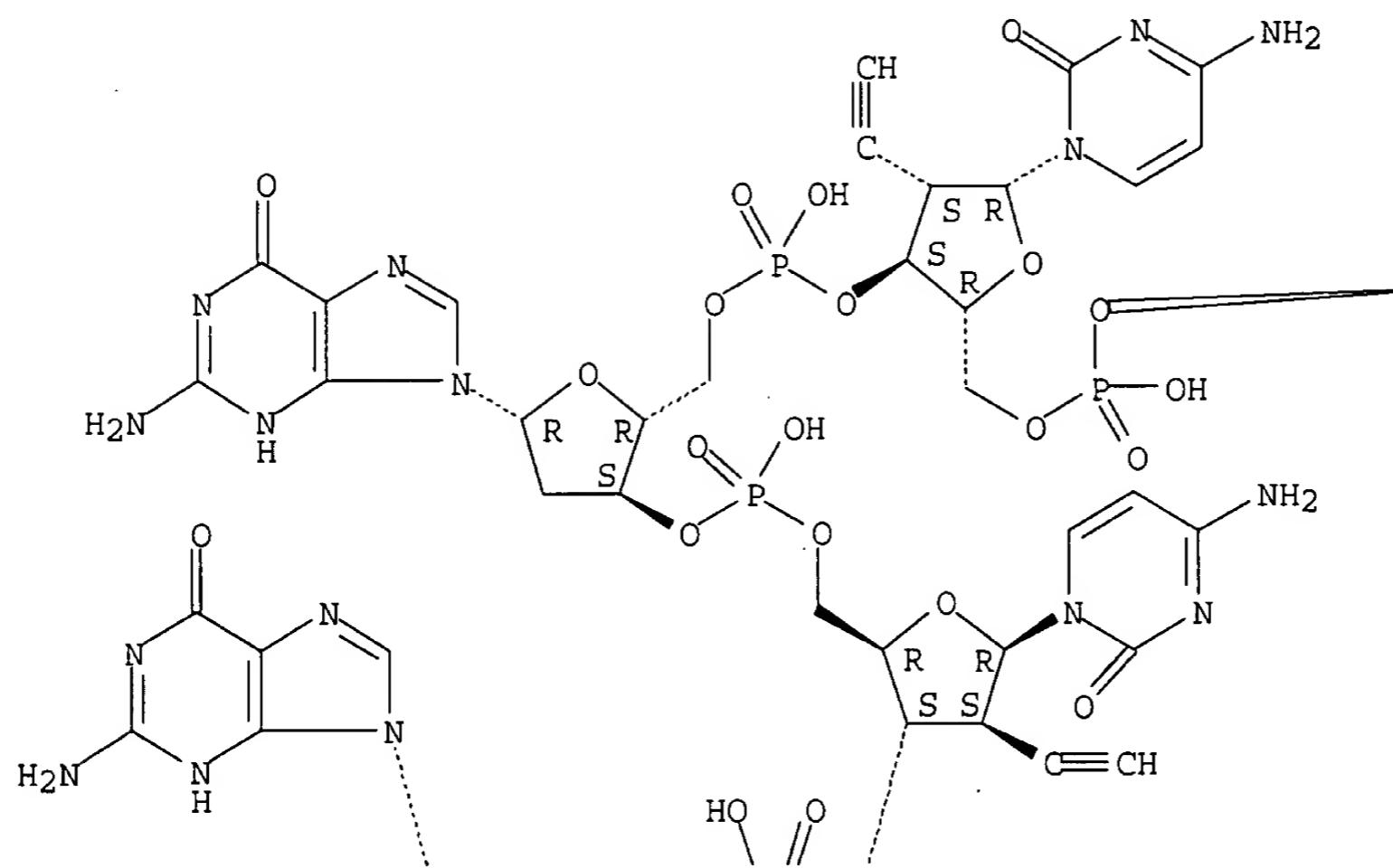
(preparation of 2'-Ethynyl-DNA to be used in the synthesis and pairing properties of DNA and RNA duplexes)

RN 231623-33-9 CAPLUS

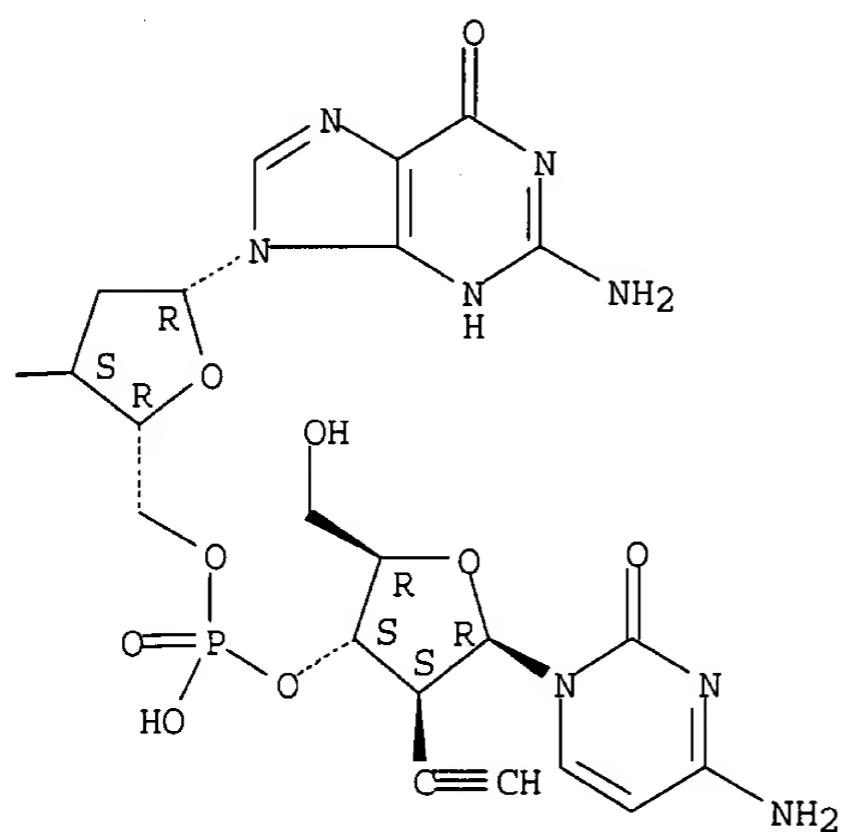
CN Guanosine, 2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

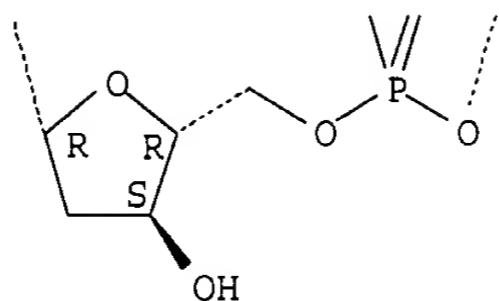
PAGE 1-A



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RN 424822-80-0 CAPLUS

CN Guanosine, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with 2'-deoxycytidylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxycytidylyl-(3'→5')-2'-deoxycytidine (1:1) (9CI) (CA INDEX NAME)

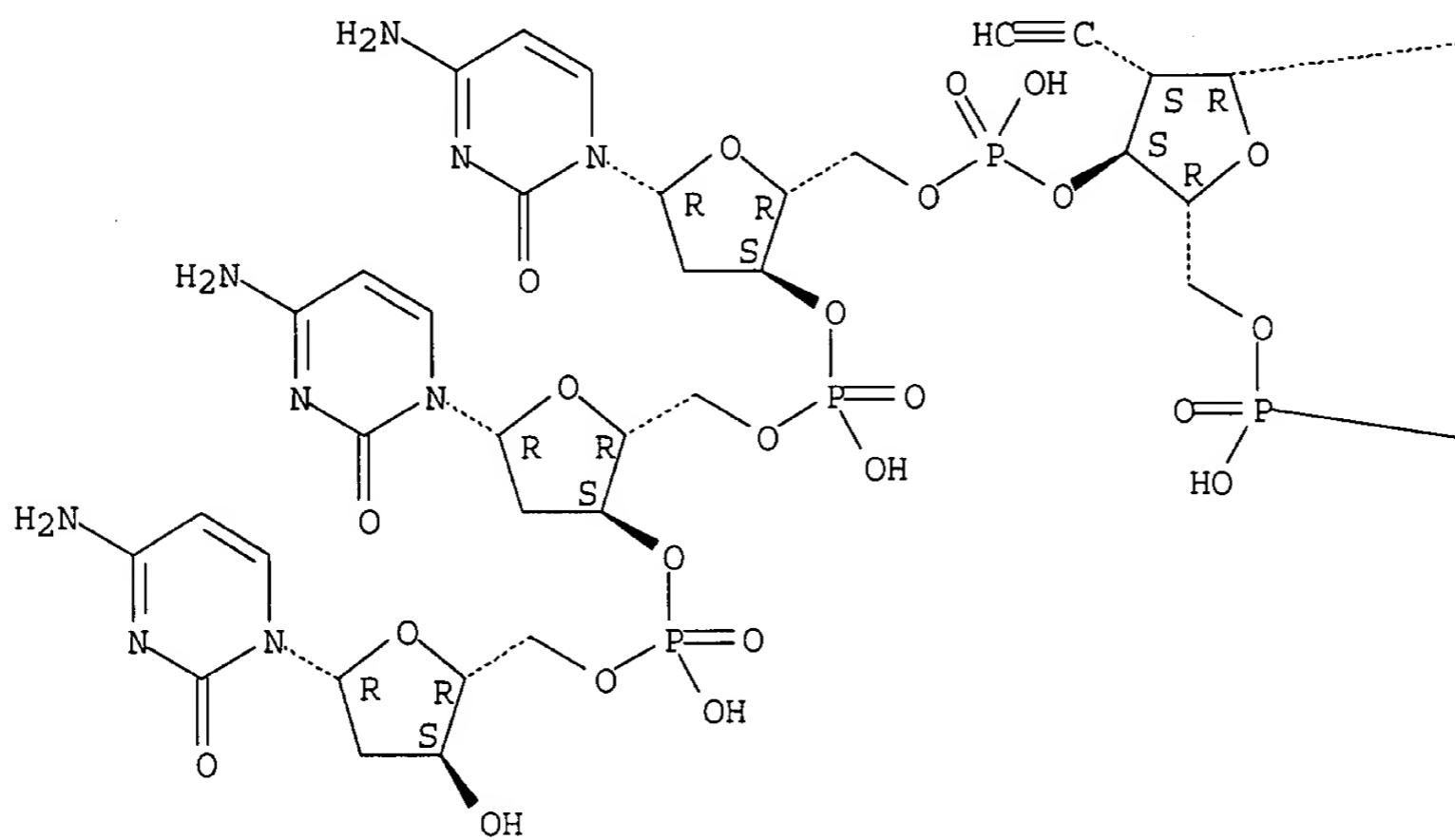
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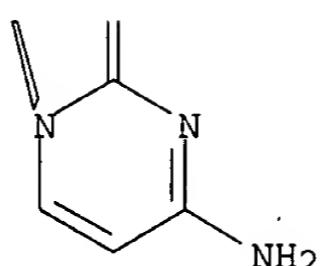
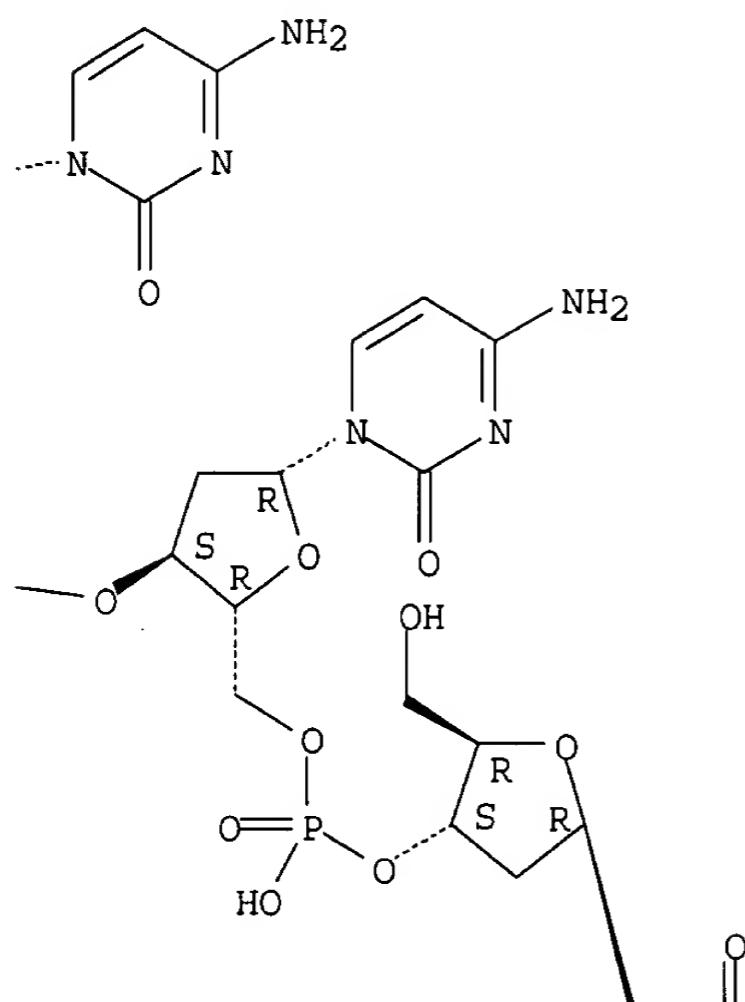
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CMF C56 H73 N18 O34 P5

Absolute stereochemistry.

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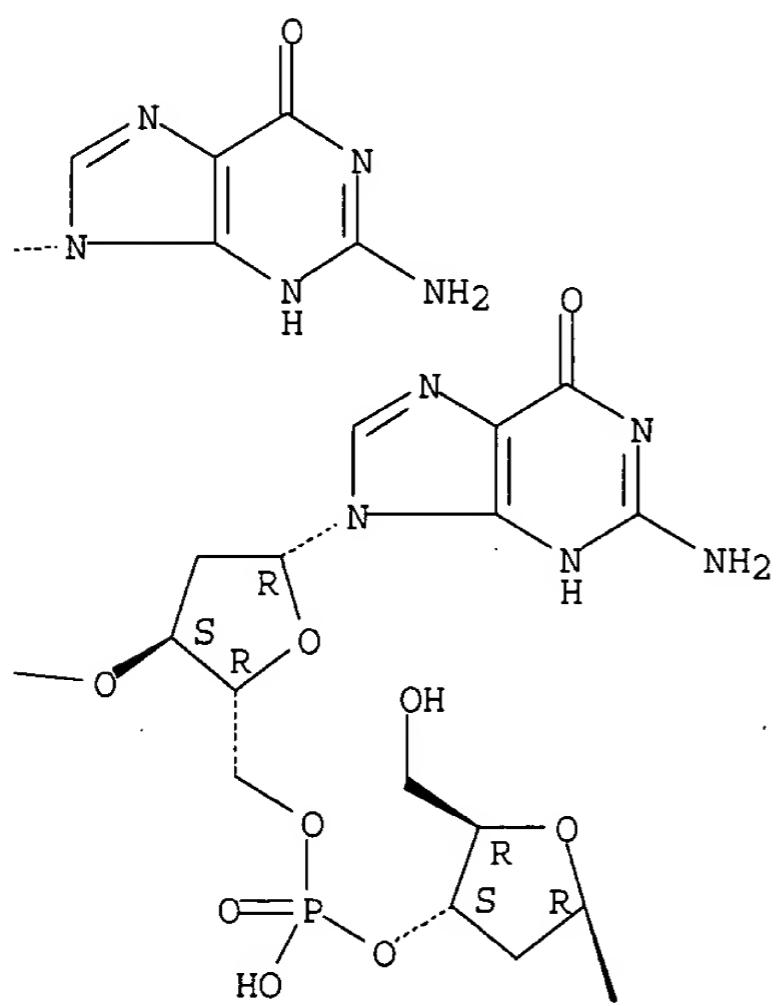
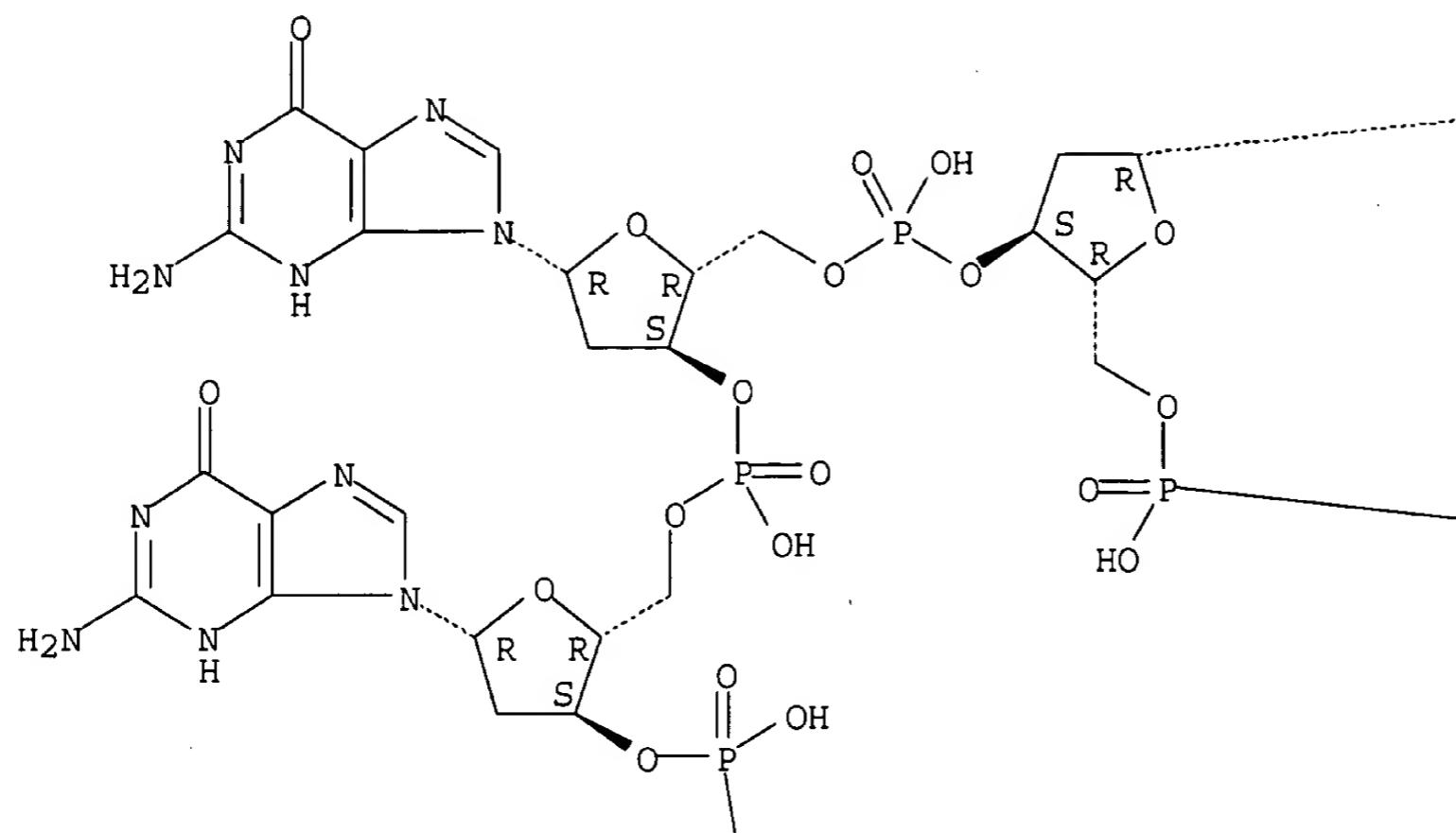




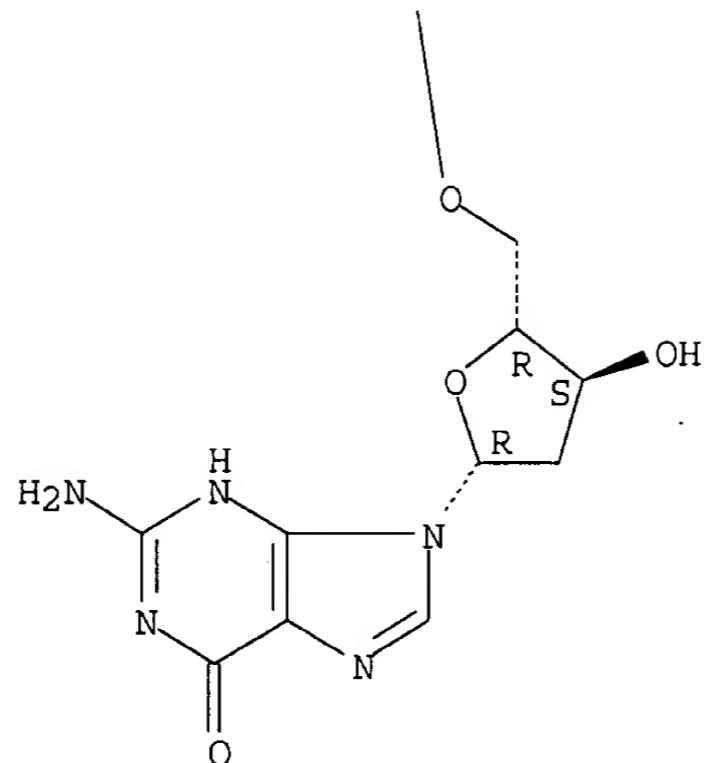
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CRN 58626-19-0  
CMF C60 H73 N30 O34 P5

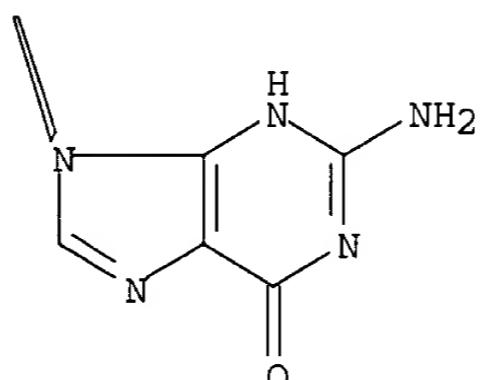
Absolute stereochemistry.



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RN 424822-82-2 CAPLUS

CN Guanosine, 2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-, complex with 2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-cytidine (1:1) (9CI) (CA INDEX NAME)

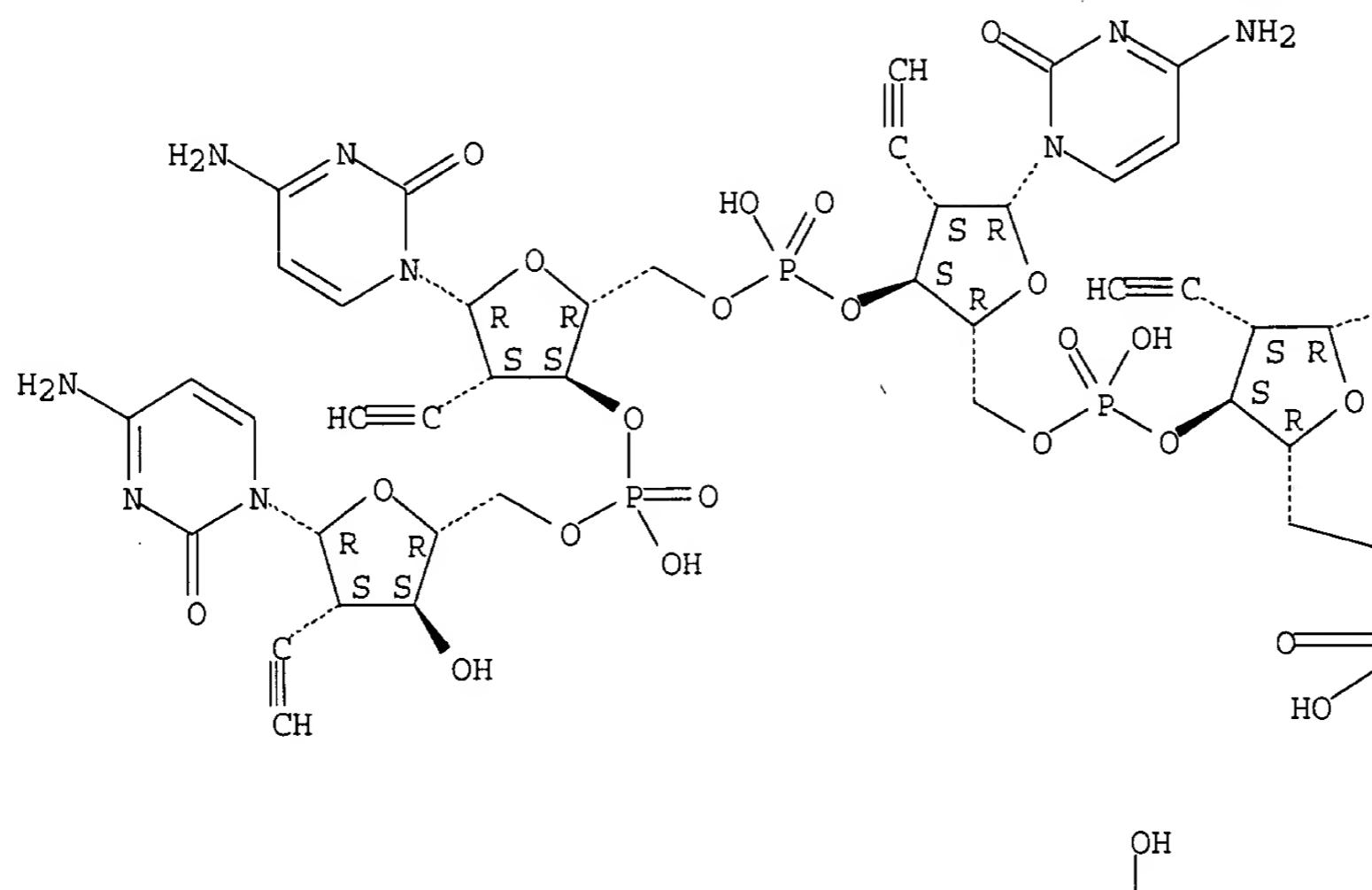
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CRN 424822-72-0

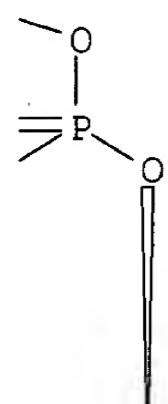
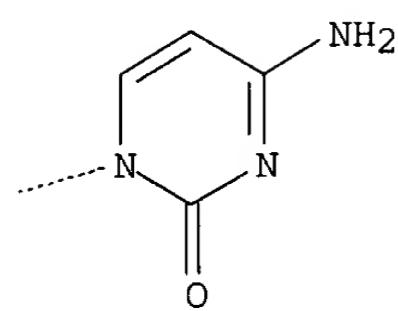
CMF C66 H73 N18 O34 P5

Absolute stereochemistry.

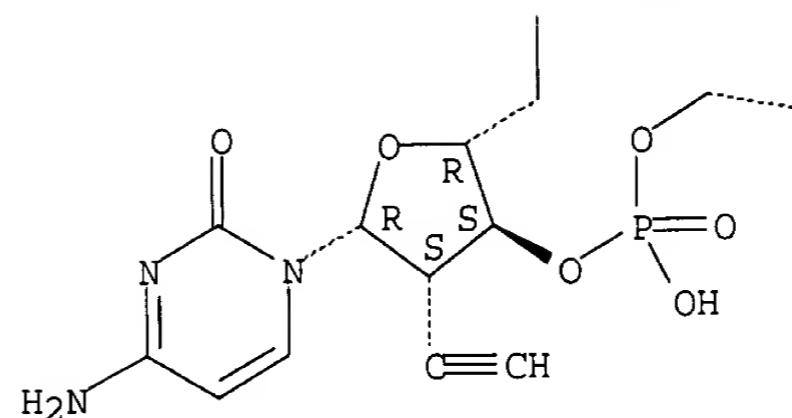
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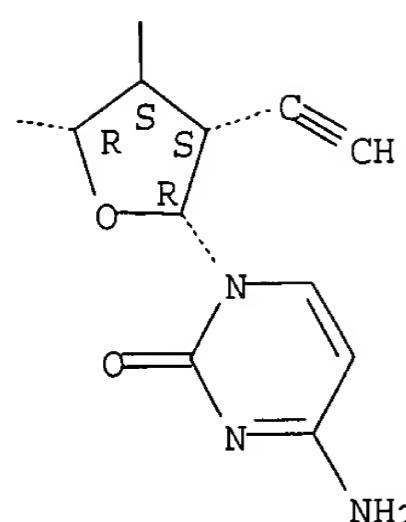
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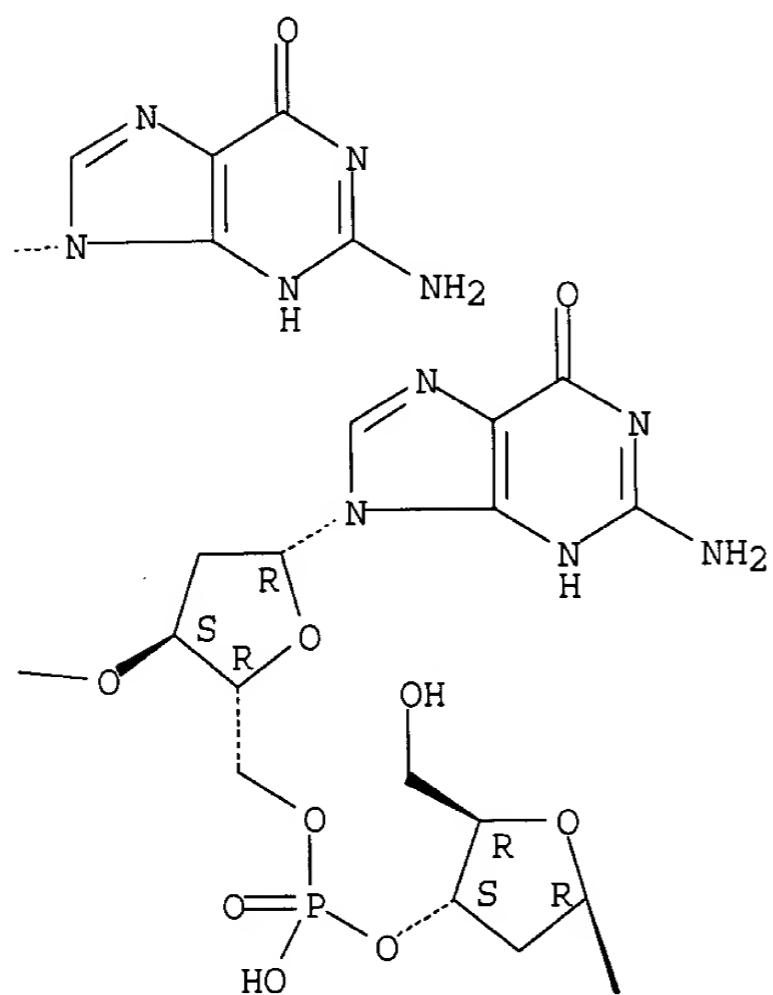
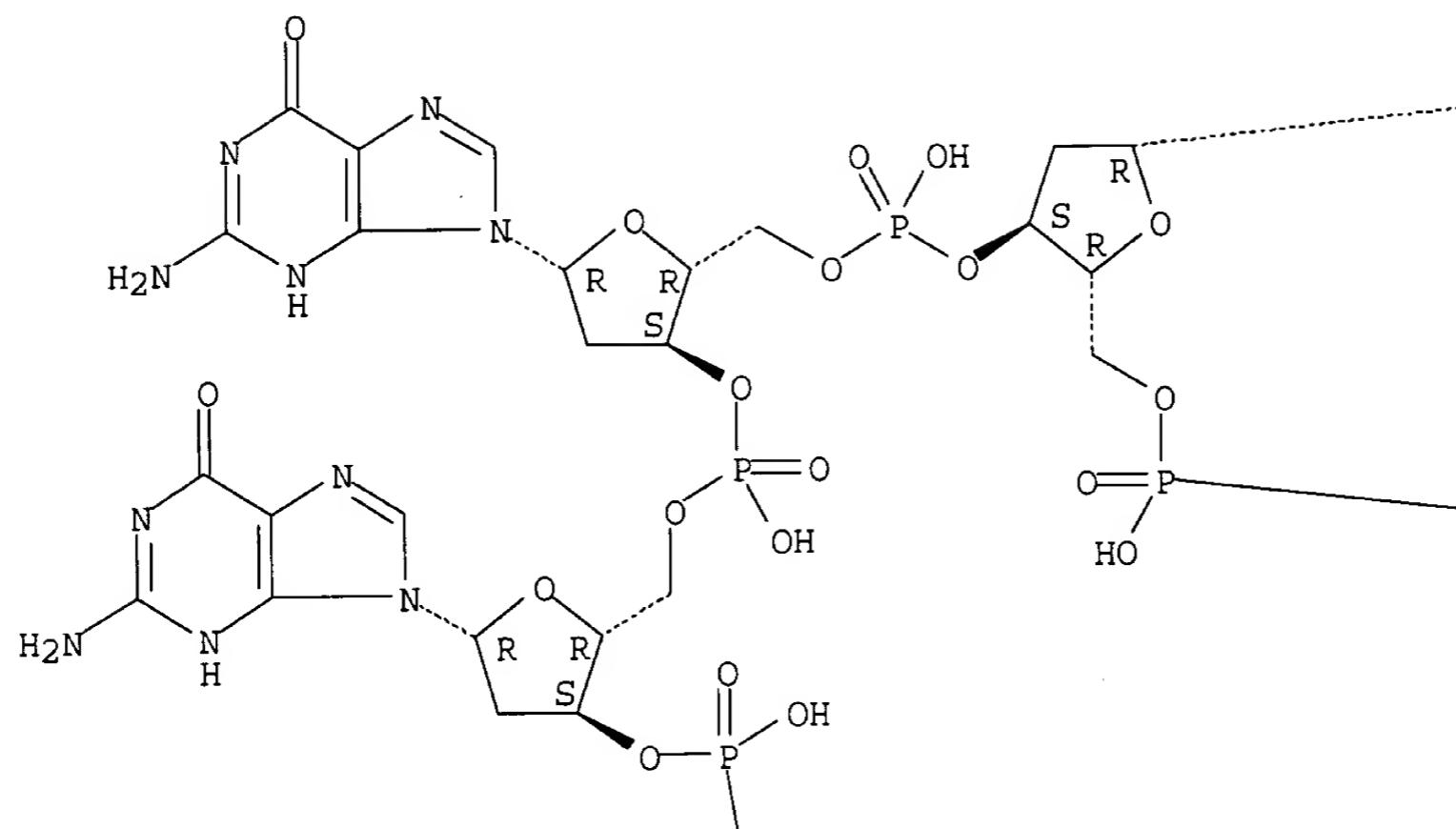
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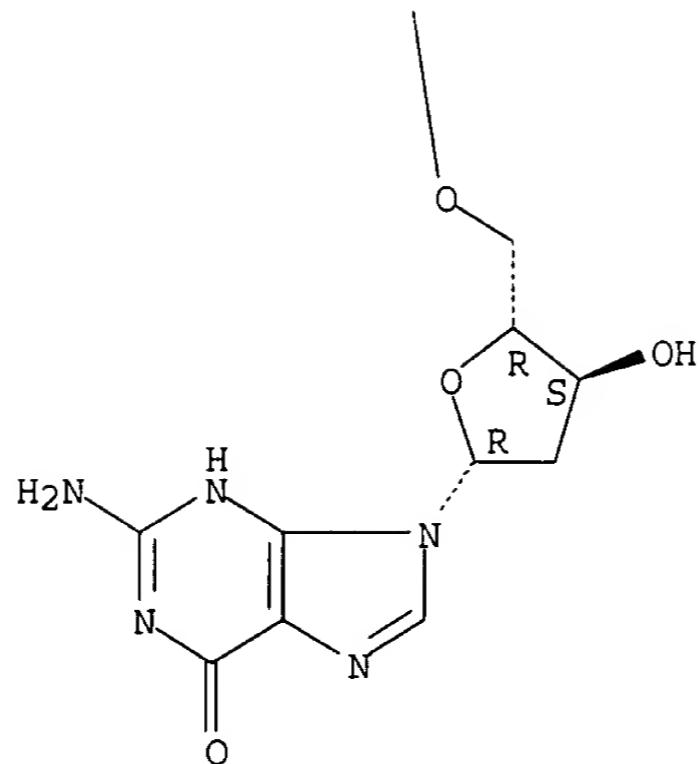
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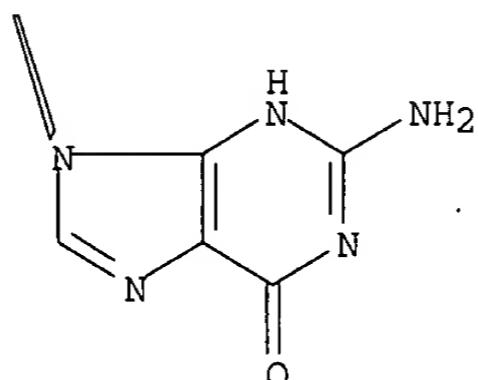
Absolute stereochemistry.



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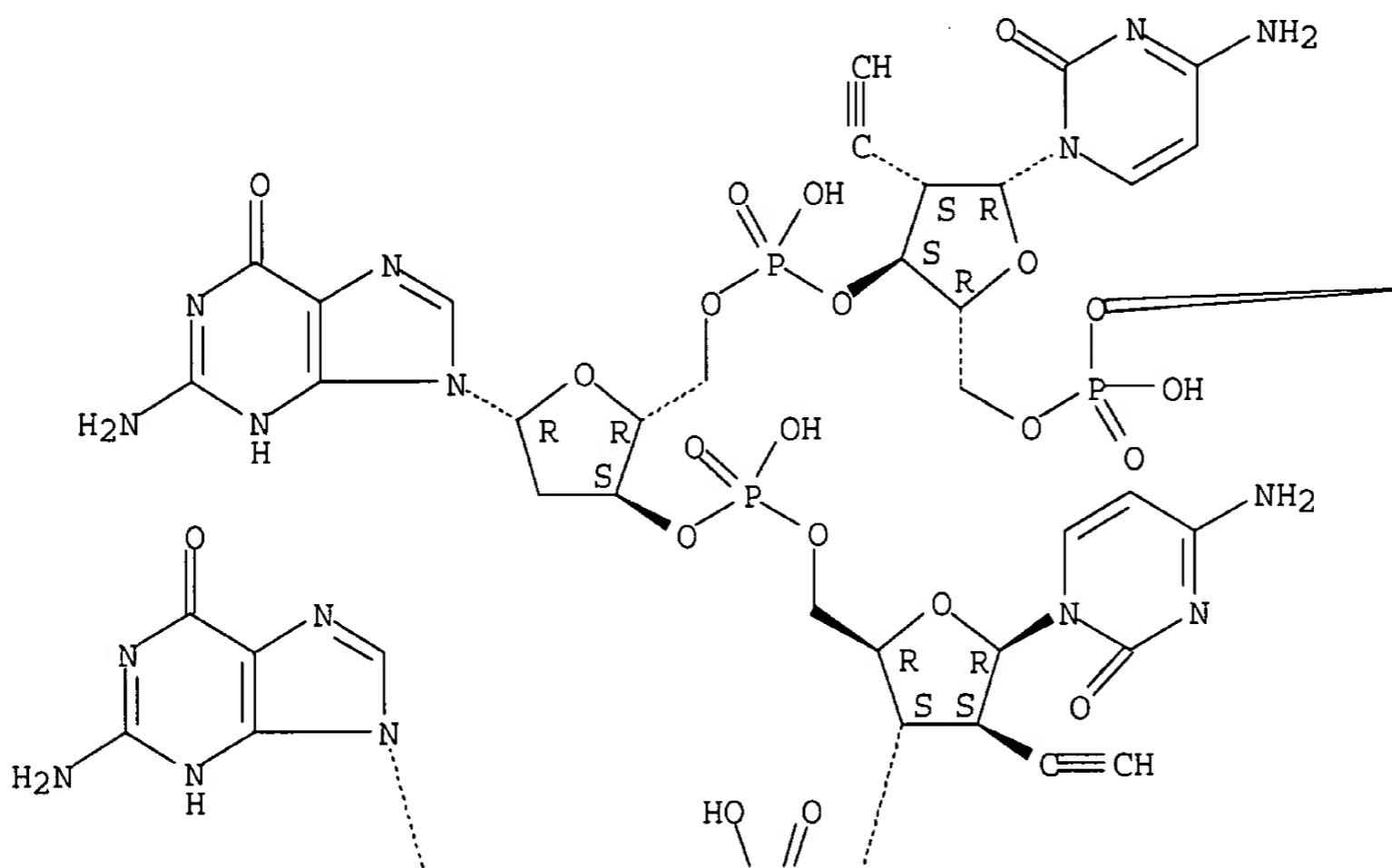
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L3 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1999:395013 CAPLUS  
 DOCUMENT NUMBER: 131:102492  
 TITLE: Z-DNA formation by 2'-C-ethynyl-modified oligonucleotides  
 AUTHOR(S): Buff, Rolf; Hunziker, Jurg  
 CORPORATE SOURCE: Department Chemistry Biochemistry, Univ. Bern, Bern, CH-3012, Switz.  
 SOURCE: Synlett (1999), (Spec.), 905-908  
 CODEN: SYNLES; ISSN: 0936-5214  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 131:102492  
 AB 9-(2'-Deoxy-2'-C-ethynyl-beta-D-arabino-pentofuranosyl)guanine phosphoramidite was prepared from guanosine in 9 steps and incorporated into oligodeoxynucleotides. Substitution of 2 or 3 ethynyl-modified guanosines for deoxyguanosine within d(CG)3 or d(GC)3 leads to a Z-DNA-like conformation of the resulting duplex regardless of salt concentration  
 IT 231623-33-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)

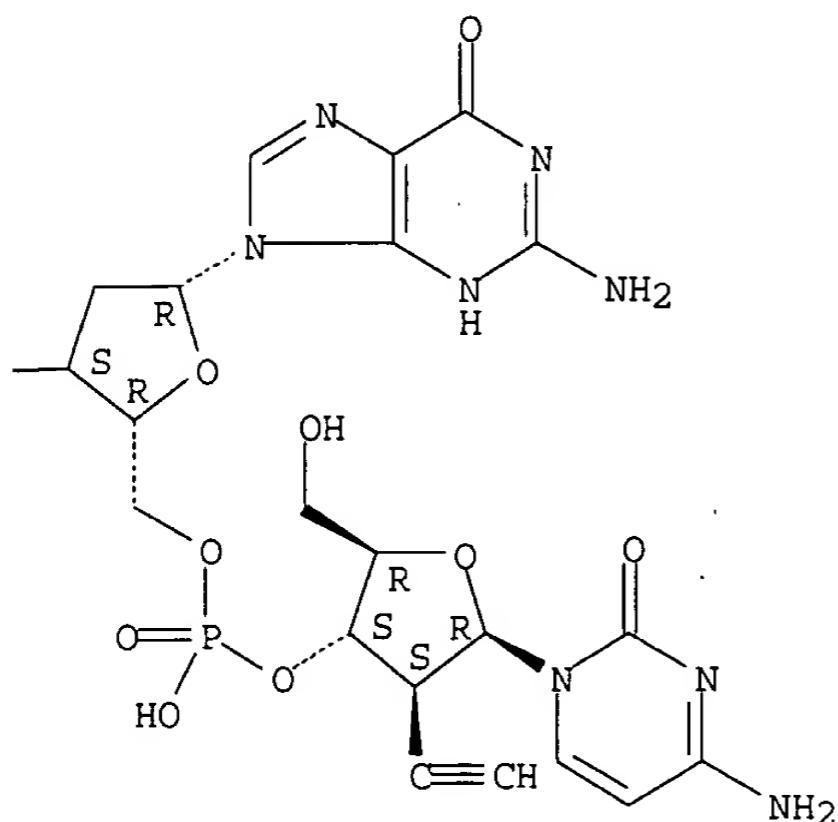
(preparation and Z-DNA formation of ethynyl-guanosine oligonucleotides)  
RN 231623-33-9 CAPLUS  
CN Guanosine, 2'-deoxy-2'-ethynyl-β-D-arabino-cytidylyl-(3'→5')-  
2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-ethynyl-β-D-arabino-  
cytidylyl-(3'→5')-2'-deoxyguanylyl-(3'→5')-2'-deoxy-2'-  
ethynyl-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry.

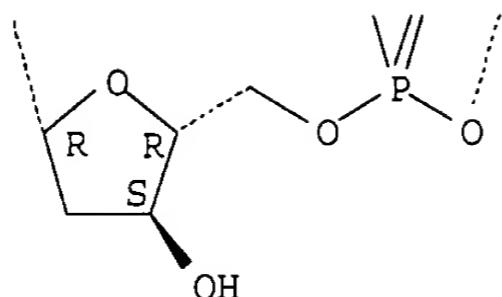
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REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:17764 CAPLUS

DOCUMENT NUMBER: 130:182710

TITLE: 2'-C-Branched Ribonucleosides: Synthesis of the Phosphoramidite Derivatives of 2'-C- $\beta$ -Methylcytidine and Their Incorporation into Oligonucleotides

AUTHOR(S): Tang, Xiao-Qing; Liao, Xiangmin; Piccirilli, Joseph A.

CORPORATE SOURCE: Howard Hughes Medical Institute Departments of Biochemistry Molecular Biology and Chemistry, University of Chicago, Chicago, IL, 60637, USA

SOURCE: Journal of Organic Chemistry (1999), 64(3), 747-754

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe a strategy for the incorporation of a 2'-C-branched ribonucleoside, 2'-C- $\beta$ -methylcytidine, into oligonucleotides via solid-phase synthesis using phosphoramidite derivs. 4-N-Benzoyl-2'-C- $\beta$ -methylcytidine was synthesized by coupling persilylated 4-N-benzoylcytosine with 1,2,3,5-tetra-O-benzoyl-2-C- $\beta$ -methyl- $\alpha$ - (and  $\beta$ ) -D-ribofuranose in the presence of SnCl<sub>4</sub> in acetonitrile, followed by selective deprotection with NaOH in pyridine/methanol. The 3' - and 5' -hydroxyl groups were blocked as a cyclic di-tert-butyldimethylsilyl ether by treatment with di-tert-butyldichlorosilane/AgNO<sub>3</sub> in DMF. The 2' -hydroxyl group was then protected as a tert-butyldimethylsilyl ether by treatment with tert-butyldimethylsilyl chloride followed by addition of tert-butyldimethylsilyl trifluoromethanesulfonate in THF. As an alternative to 2'-silyl protection, the corresponding 2'-O-tetrahydropyranyl ether was prepared by treatment with 4,5-dihydro-2H-pyran in the presence of a catalytic amount of 10-camphorsulfonic acid in methylene chloride. The di-tert-butyldimethylsilyl groups were removed by treatment with pyridinium poly(hydrogen fluoride). Protection of the 5' -hydroxyl group as a dimethoxytrityl ether and phosphitylation of the 3' -hydroxyl group by the standard procedure gave the phosphoramidite derivs. Both these derivs. could be used to incorporate 2'-C- $\beta$ -methylcytidine into oligonucleotides efficiently via standard solid-phase synthesis, but the tetrahydropyranyl group was more readily removed from oligonucleotides than the tert-butyldimethylsilyl group. Oligonucleotides containing 2'-C- $\beta$ -methylcytidine undergo base-catalyzed degradation analogous to natural RNA.

IT 220503-72-0P 220503-75-3P 220503-77-5P

220503-93-5P 220503-95-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

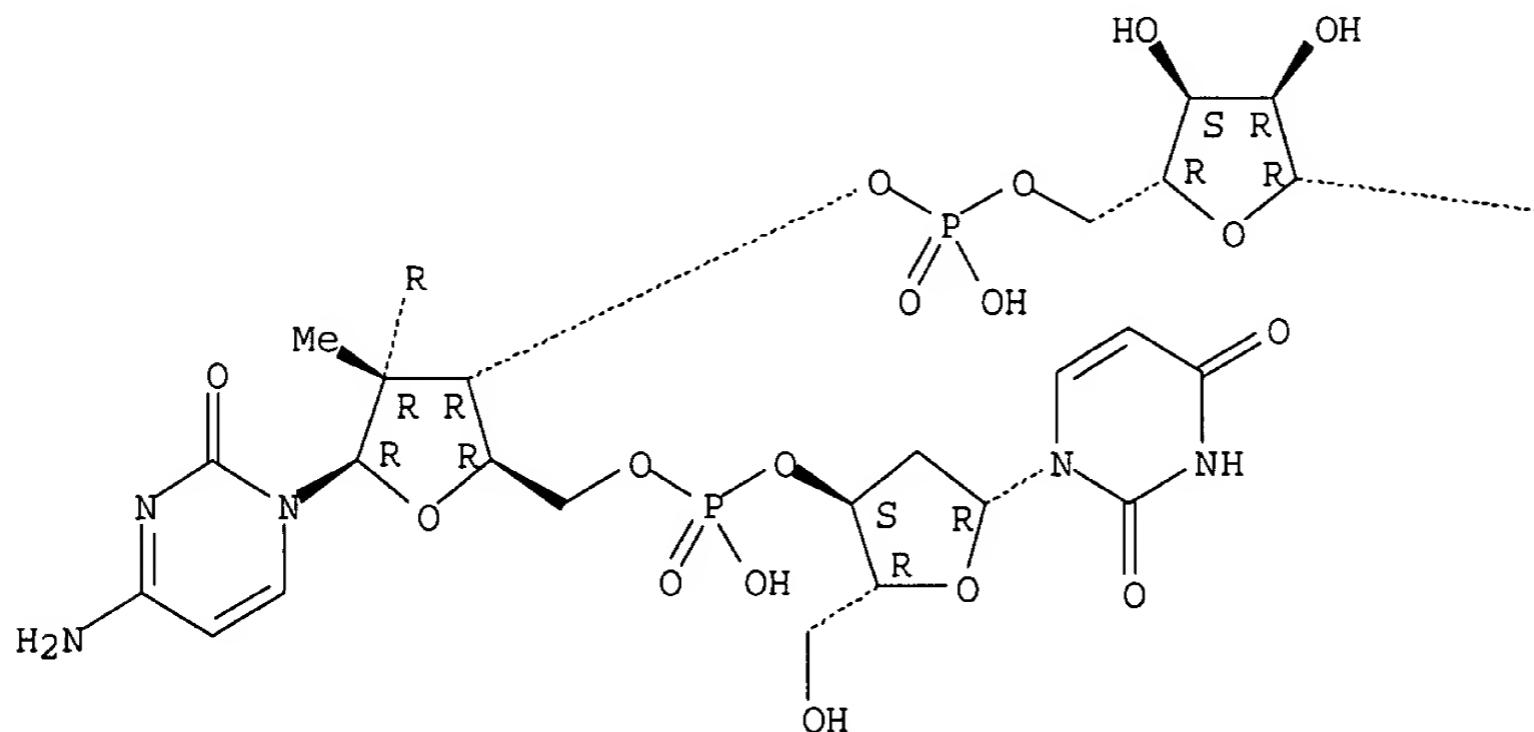
(preparation of the phosphoramidite derivs. of 2'-C- $\beta$ -methylcytidine and their incorporation into oligonucleotides)

RN 220503-72-0 CAPLUS

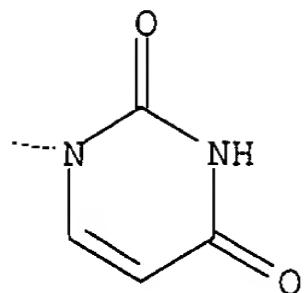
CN Uridine, 2'-deoxyuridylyl-(3'  $\rightarrow$  5')-2'-O-[(1,1-dimethylethyl)dimethylsilyl]-2'-C-methylcytidylyl-(3'  $\rightarrow$  5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

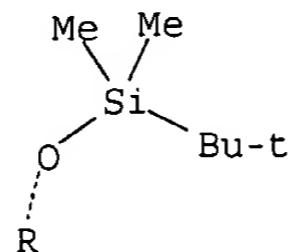
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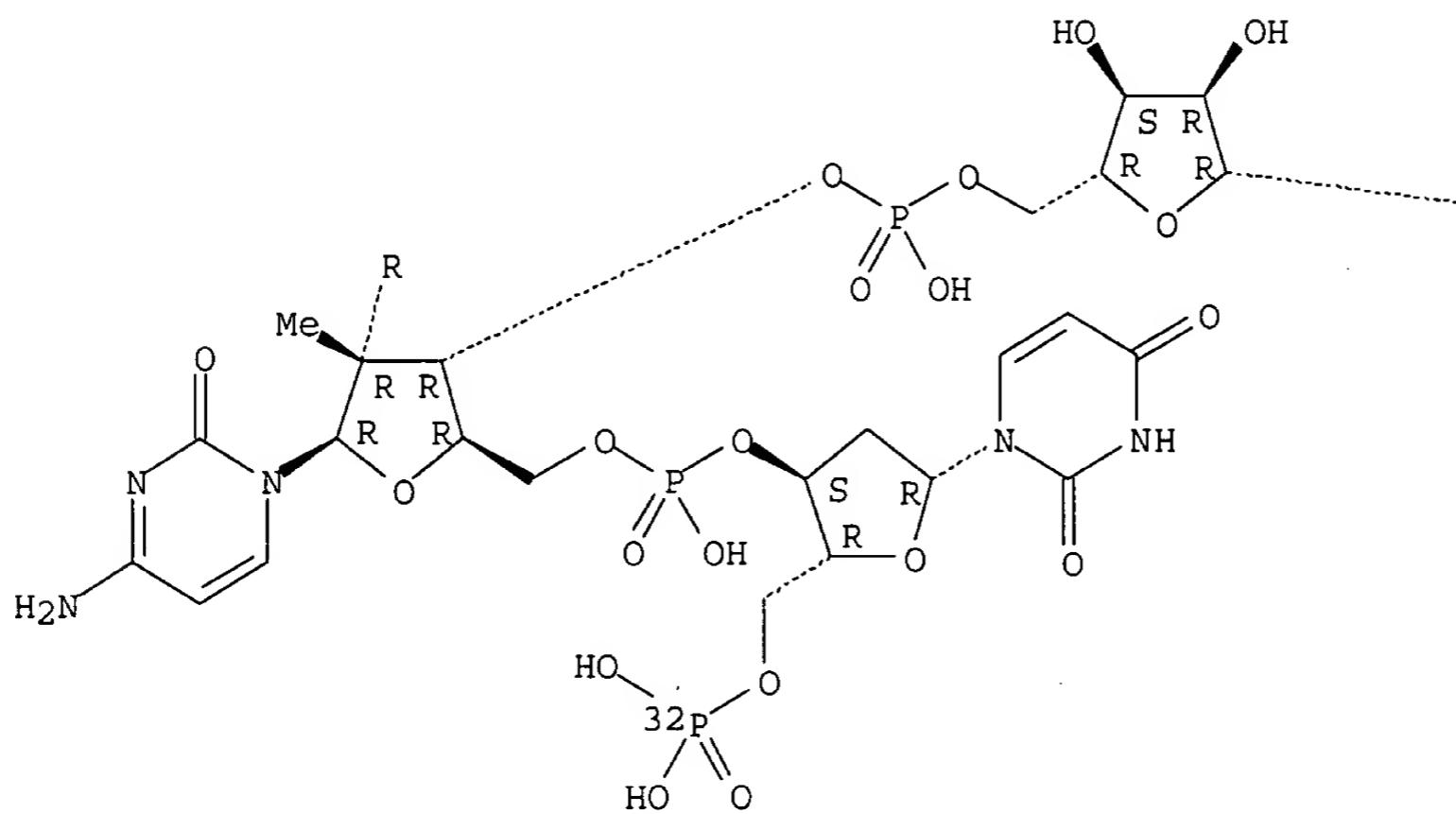


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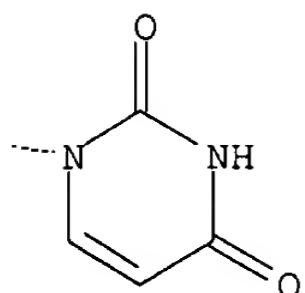
CN Uridine, 2'-deoxy-5'-O-(phosphono-32P)uridylyl-(3'→5')-2'-O-[(1,1-dimethylethyl)dimethylsilyl]-2'-C-methylcytidylyl-(3'→5')- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

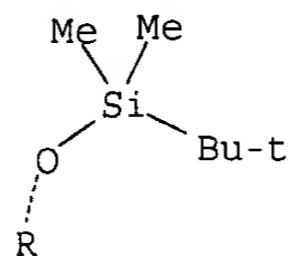
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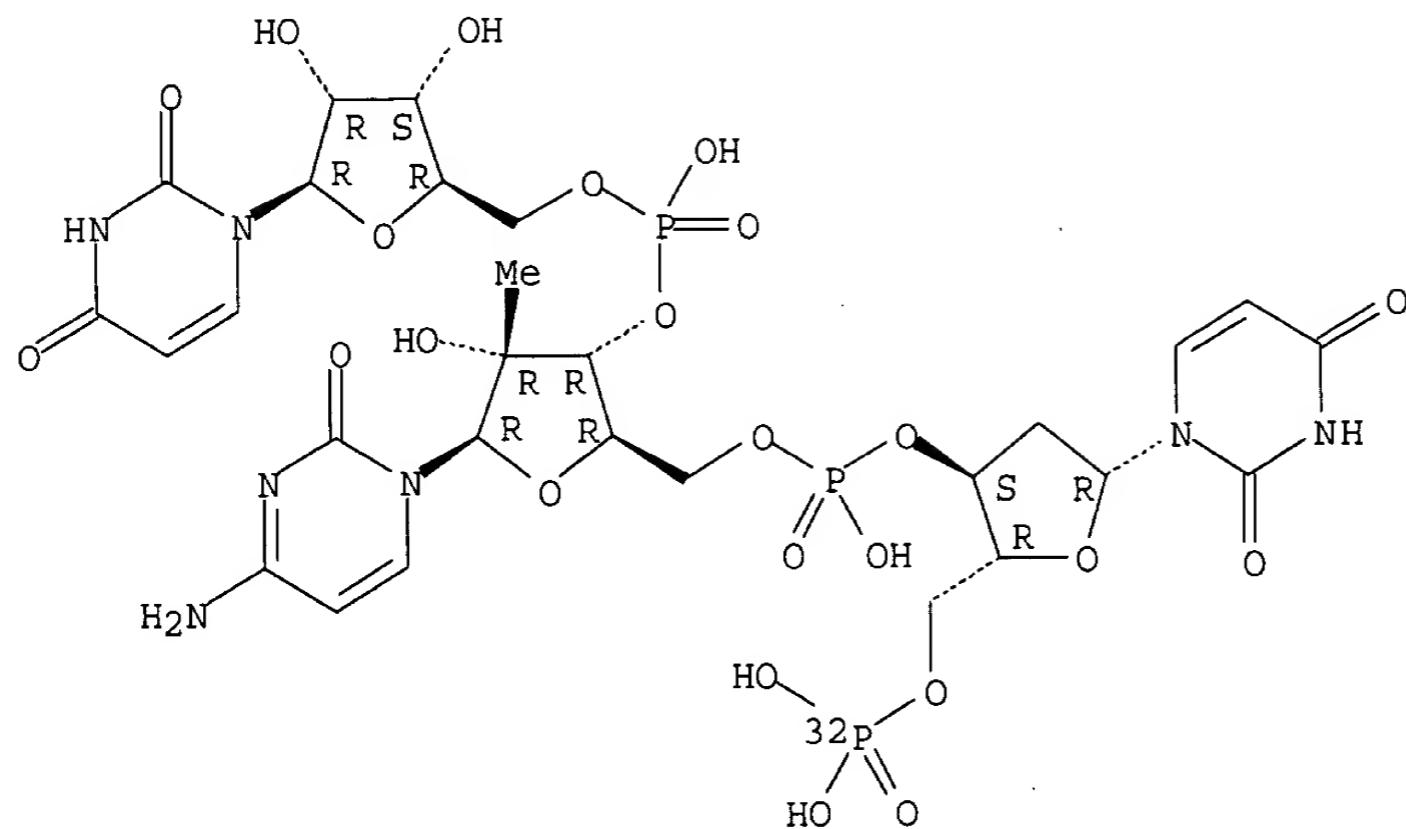
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RN 220503-77-5 CAPLUS

CN Uridine, 2'-deoxy-5'-O-(phosphono-32P)uridylyl-(3'→5')-2'-C-methylcytidylyl-(3'→5')- (9CI) (CA INDEX NAME)

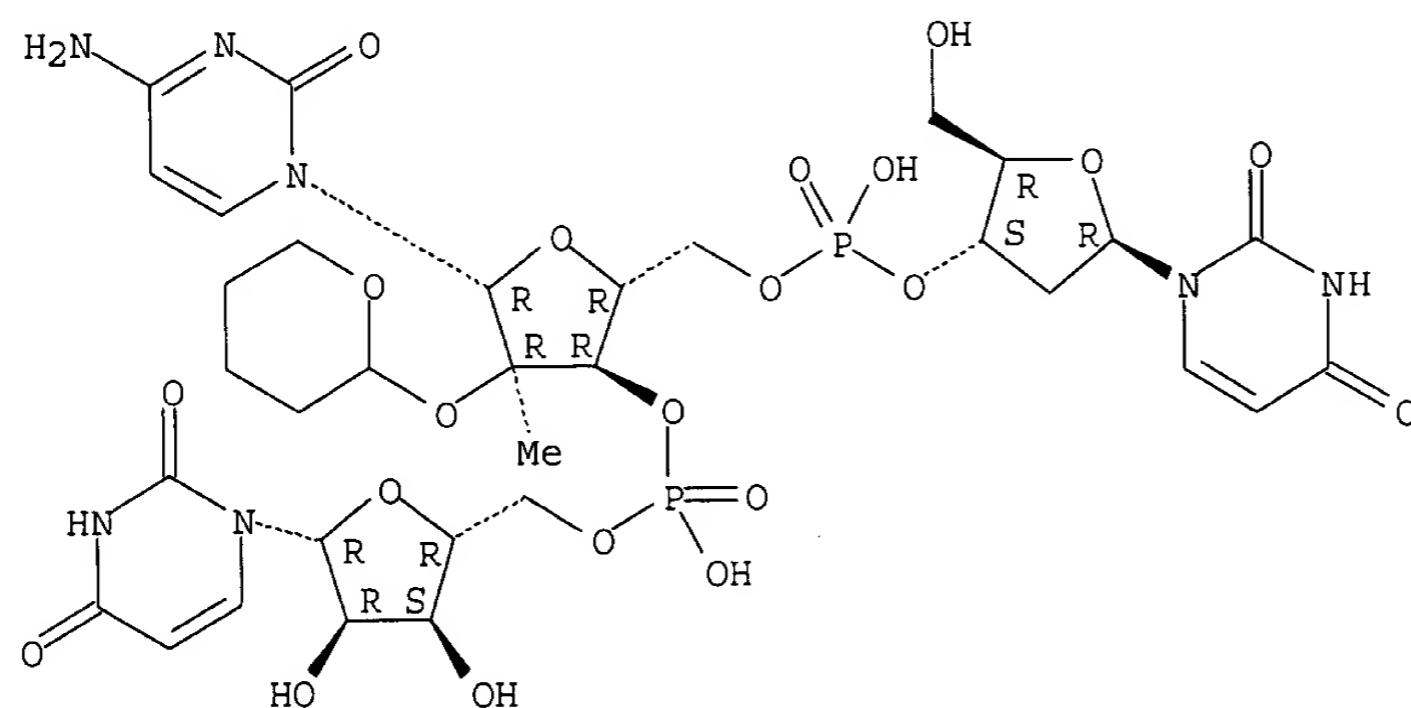
Absolute stereochemistry.



RN 220503-93-5 CAPLUS

CN Uridine, 2'-deoxyuridyl-(3'→5')-2'-C-methyl-2'-O-(tetrahydro-2H-pyran-2-yl)cytidyl-(3'→5')- (9CI) (CA INDEX NAME)

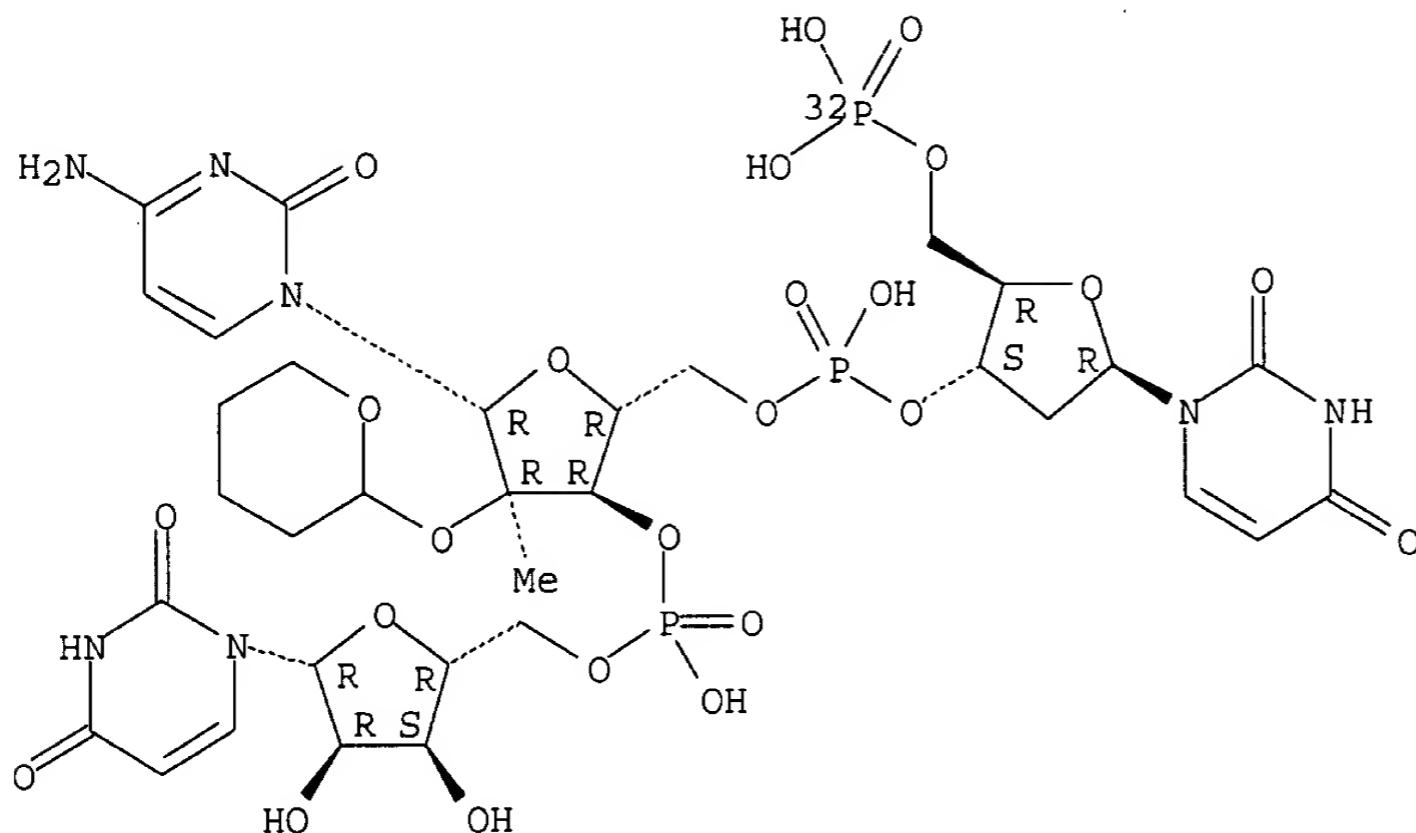
Absolute stereochemistry.



RN 220503-95-7 CAPLUS

CN Uridine, 2'-deoxy-5'-O-(phosphono-32P)uridyl-(3'→5')-2'-C-methyl-2'-O-(tetrahydro-2H-pyran-2-yl)cytidyl-(3'→5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

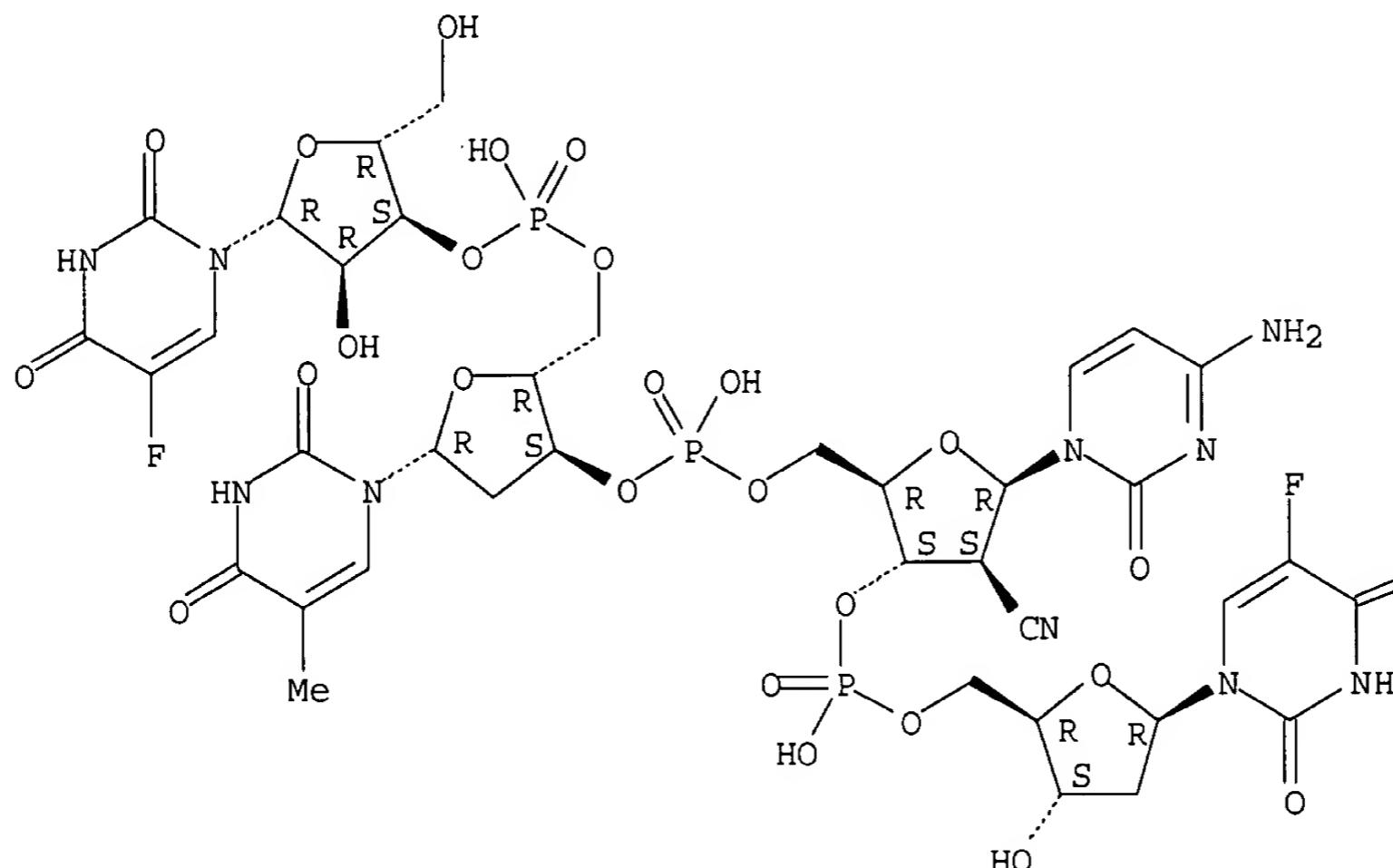
L3 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1998:535791 CAPLUS  
 DOCUMENT NUMBER: 129:276238  
 TITLE: Preparation of oligonucleotides having 5-fluorouracil moiety  
 INVENTOR(S): Ozaki, Shoichiro  
 PATENT ASSIGNEE(S): Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10218893	A2	19980818	JP 1994-308073	19941107
PRIORITY APPLN. INFO.:			JP 1994-308073	19941107
AB Oligonucleotides having $\geq 1$ 5-fluorouracil moiety, useful as antitumor agents with reduced cytotoxicity, are prepared by binding 5-fluorouridine or 5-fluoro-2'-deoxyuridine 5- or 3-(cyanoethyl phosphoramidite) or 2-(chlorophenyl phosphate) with nucleotides. IC50 of 5-fluorouridylyl-(5' $\rightarrow$ 5')-5-fluorouridine, prepared from 2',3'-O-isopropylidene-5-fluorouridine and $\beta$ -cyanoethyl phosphorodichloridite with 3 steps, against growth of human gastric cancer cell KATO-III was 0.005 $\mu$ M, vs. 0.021 $\mu$ M of 5-fluorouracil.				
IT 214000-75-6P 214000-76-7P	RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of oligonucleotides having 5-fluorouracil moiety as antitumor agents)			
RN 214000-75-6 CAPLUS				

CN Uridine, 5-fluorouridylyl-(3'→5')-thymidylyl-(3'→5')-2'-cyano-2'-deoxy-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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PAGE 1-B

$\equiv O$

RN 214000-76-7 CAPLUS

CN Uridine, 2'-deoxy-5-fluorouridylyl-(3'→5')-2'-cyano-2'-deoxy-β-D-arabino-cytidylyl-(3'→5')-2'-deoxy-5-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

